# Strategic Plan IQCC 2024-2026

# TABLE OF CONTENTS


**PREAMBLE** 5

**INTRODUCTION** 7

**Mission** 7

**Vision** 8

**Values** 8

**Brief history of the IQCC** 8

**A comparison of IQCC with similar Institutes** 8

**STRATEGIC AIMS** 10

**Education** 10
Master in Advanced Catalysis and Molecular Modelling (MACMoM) 11
Doctoral training 11

**Research** 12
Open Science, FAIR Data 13

**Societal Impact** 14
Collaboration with industry 14
Technology transfer 14
Science communication 15
Collaboration with the C4D unit 16

**INTERNATIONALIZATION** 16

**HUMAN CAPITAL** 17

**General talent attraction and retention** 17

**BSc/MSc students** 18

**PhD students** 18

**Postdocs** 18

**Support staff** 19

**Staff** 19

**Promotion of gender equality** 20

**GOVERNANCE** 20

**INFRASTRUCTURE** 23

**Housing** 24

# Preamble

The third Strategic Plan of the Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona (UdG) is presented below, which has been drawn up by the members of the IQCC and approved by the Council of the IQCC. The first Strategic Plan of the IQC was approved by the IQCC Council for the period 2005-07 on 11th March 2005. There was a second Strategic Plan of the IQCC for the period 2015-2018 that was approved on 10th June 2015. The current Strategic Plan must mark the lines of action mainly for the next three years, although in some cases the proposed actions can be extended for several more years.

When I was elected director of the IQCC, there was an already very advanced version of this Strategic Plan. I want to acknowledge the work carried out by the previous director, Prof. Marcel Swart and the commission that was created to write the second Strategic Plan of the IQCC whose members were Prof. Marcel Swart, Prof. Miquel Costas, Prof. Lluís Blancafort, Prof. Anna Roglans, Dr. Ferran Feixas, and Dr. Teresa Corona, as well as all members of the IQCC that proposed additions and changes to the first drafts of this Strategic Plan.

This Strategic Plan identifies the strengths and weaknesses of the IQCC to establish, based on an analysis in the form of possible problems and opportunities, the actions to be developed to improve the organization of the center, the research results, and the contributions that the IQCC can make to society. Most of the data of this Strategic Plan were collected by Dr. Teresa Corona when writing the María de Maeztu 2023 application.

In this plan, the IQCC's strategic reflection is drawn up and concreted into government actions that will have to be developed in the next three years. It is clear that everyone's effort will be needed to move forward: the effort of the technical and administrative staff to be effective in their management and maintenance tasks and to facilitate the work of IQCC researchers; the effort of doctoral students to enthusiastically develop their research, offer their help in the various events organized by the IQCC, and facilitate the integration of undergraduate students who join the Institute; the effort of senior researchers and post-docs to direct part of their research in a direction that facilitates the achievement of the objectives proposed here, to invite young and established researchers of recognized prestige to help us maintain a high level of research and to renew our knowledge, and also to request projects that allow us to enjoy the funding that the IQCC needs to carry out its research: and finally, the effort of the management team to maintain the course that this Plan sets for us. With everyone's effort, I am sure that we will achieve the milestones proposed in this Plan.

Miquel Solà
Director

# Introduction

In April 2023, the IQCC celebrated its thirtieth anniversary in Girona, having gone from a small group of researchers to three consolidated research groups that have been recognized by the Generalitat de Catalunya early 2023. At the end of the 2022-23 academic year, the institute consisted of 104 researchers (6 full professors, 9 associate professors, 2 ICREA Senior researchers, 2 Ramón y Cajal researchers, 3 ex-professors, 24 postdocs, 58 PhD students) and 6 support staff (1 research manager, 3 technicians, 2 administrative staff). This is the result of a steady and consistent growth in the number of funded research projects, research fellowships, and human capital. Since joining forces in 2013 with the experimental groups in organic and bioinorganic/supramolecular chemistry, the institute produced a total of 61 PhD theses. Researchers are grouped into three main research groups, all of which are recognized and funded by the Government of Catalonia in its 2021 consolidated group call (SGR-Cat 2021): the Bioinspired, Supramolecular, and Catalysis Chemistry Group (QBIS-CAT) with 4 principal investigators, the Design and Modeling of Transition Metal-Catalyzed Reactions Group (DiMoCat) with 6 principal investigators, and the Theoretical Chemistry of Biosystems Group (TCBioSys) with 5 principal investigators. On average, during the period 2019-2022, the Institute has received an annual funding of 2.3 M€, most of which comes from competitive European or National Plan calls. The productivity of the IQCC is supported by the publication of 470 articles (402 Q1, 250 D1) during the period 2018-2022, which have received more than 7500 citations. Some of these articles have been published in journals such as Science, Nature, Nature Chem., Chem, JACS, ACIE, etc. In the same period, 29 doctoral theses have been defended, 18 of which have international mention and 10 were foreign PhD students. Finally, the IQCC, through the Chair of Scientific Culture and Digital Communication (C4D), has carried out a very important task of scientific communication, being the annual organization of the Night of Research since 2008 one of its most outstanding activities.

*Members of the IQCC, December 2022.*

## Mission

The IQCC aims to improve society by advancing towards a more sustainable and innovative society through science, education, and research. The IQCC operates internationally and uses synergistic cooperation between theoretical and experimental teams to address scientific global challenges ligated to chemical sciences, expanding the limits of knowledge and providing innovative solutions. Research is naturally connected with the training of young

generations of scientists, and the education of UdG students of multiple disciplines. Moreover, the institute is a major contributor to the scientific education of the local environment while also contributing to its development. In particular, the industrial and educational sectors benefit from institute outputs in terms of trained individuals and scientific knowledge that fuels innovation and promotes their competitiveness.

## Vision

We envision the IQCC as a leading institute of chemistry in Catalonia and Spain, gradually positioning itself at the forefront of the European Research Area. The institute is based on an open minded academic community that provides opportunities for students, postdocs, support staff, and research staff to develop themselves and grow towards becoming leaders in their field. Our researchers are curious, tackling chemical problems from a variety of viewpoints and expertise, often complementary, from both a computational and experimental background.

## Values

We strive for the highest standards of integrity and intellectual and creative excellence. We value originality, honesty, audacity, and the free exchange of ideas and information. We love discovery and exploration and challenge our assumptions and absorb knowledge from others with fearless curiosity. We work hard to make our Institute a kind and inclusive environment where people from various backgrounds can develop and where everyone has a sense of belonging.

## Brief history of the IQCC

IQCC is a university research institute created in accordance with Law 26/1984 of the Parliament of Catalonia. The initial seed of the Institute was the so-called Laboratory of Computational Chemistry (LQC) of the UdG, which started its activity before the official creation of UdG on December 31, 1991. On July 6, 1992, the Management Committee of UdG agreed to initiate the legal procedure for the creation of the Institute of Computational Chemistry (IQC). Finally, the IQC officially began its trajectory on March 30, 1993, in a meeting of the provisional Council of the Institute chaired by the president of the UdG management committee at that time, Prof. Dr. Josep Nadal. On April 20, 1993 (official date of creation of the IQC), the president of the management committee (equivalent to rector), Prof. Dr. Josep Nadal, appointed Prof. Dr. Ramon Carbó-Dorca as the first director of the IQC, a position he held until 2004. Subsequently, the institute has been directed by Profs. Miquel Solà (2004-2007), Lluís Blancafort (2007-2015), and Marcel Swart (2015-2023). During the mandate of Prof. Blancafort, the current IQCC was created by joining the groups of the IQC with the groups of Bioinorganic and Supramolecular Chemistry and Transition Metals in Organic Synthesis, both from the Department of Chemistry at UdG. The Governing Council in session 1/2013, on February 27, 2013, approved the change of name from Institute of Computational Chemistry to Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona, as well as its regulations (BOUdG no. 2/2013, of March 14, 2013). Likewise, the Governing Council in session 5/2013, on September 25, 2013 (BOUdG no. 5/2013, of October 14, 2013) and in session 2/2023, on February 27, 2023 (BOUdG no. 2/2023, of March 14, 2023) approved the modification of the regulations to adapt them to different regulatory changes.

## A comparison of IQCC with similar Institutes

In order to place the performance of IQCC in a European context, research outcomes of the IQCC in the recent five-year period of 2018-2022 are compared with five European Institutes of similar size and interests. In particular, the Institutes analyzed are the Stratingh Institute for Chemistry (Univ. Groningen, Netherlands), the Hylleraas Centre for Quantum Molecular Sciences (Norway), the Institut de Science et d'Ingénierie Supramolécularires (ISIS, France), the Institute of Theoretical and Computational Chemistry (IQTC) of the Universitat de Barcelona, and the Institute of Molecular Science (ICMol) of the Universitat de València.

The mission of the Stratingh Institute for Chemistry (Univ. Groningen) is to perform excellent research and teaching in molecular and supramolecular chemistry. Core activities in the chemical sciences such as bio-organic chemistry, organic chemistry, molecular inorganic chemistry, and molecular materials chemistry are embedded in

the institute. The research program is focused on synthesis, catalysis, functional materials, bio-organic chemistry/chemical biology, and systems chemistry/complex molecular systems. The Stratingh Institute is currently employing 18 permanent researchers, 30 postdocs, and 98 PhD students, for a total of 146 researchers. Together with administrative and secretarial support (8 in total), the institute is considerably larger than the IQCC. There is no publicly available information on the budget of the institute.
Source of information: https://www.rug.nl/research/stratingh/?lang=en + Scopus with search affiliation = Stratingh and affiliation city = Groningen

The Hylleraas Centre for Quantum Molecular Sciences is a Norwegian Centre of Excellence shared equally between the University of Oslo and the University of Tromsø - The Arctic University of Norway, with the University of Oslo as project owner. It receives an annual funding of 15 million NOK (1000 NOK ≈ 85 EUR) from The Research Council of Norway, plus additional substantial support from the host institutions (Univ. Oslo, Univ. Tromsø). The Hylleraas Centre was established on 1st October 2017 for a period of 5 years with the possibility of an extension for a further 5 years following a mid-term evaluation. It employs 7 Principal Investigators, 19 senior researchers, 9 postdocs, 32 PhD students, and 7 administrative and technical staff at the end of 2022.
Source of information: https://www.mn.uio.no/hylleraas/english/about/ + Scopus with search affiliation = Hylleraas and affiliation city = (Oslo OR Tromso)

The Institut de Science et d'Ingénierie Supramolécularires (ISIS) is a Mixed Research Unit (UMR 7006) of CNRS and the University of Strasbourg. Its mission is to do multidisciplinary research at the interface between Physics, Chemistry, and Biology. To this end, the institute is located at the Esplanade campus (in the center of Strasbourg), surrounded by the faculties of Physics, Chemistry, and Life Sciences. It employs 18 Principal Investigators (including two Nobel Prizes, Jean-Marie Lehn (1987) and Jean-Pierre Sauvage (2016)), 23 senior researchers, 49 postdocs, 93 PhD students, and 8 administrative and technical staff at the end of 2022. There is no publicly available information on the budget of this institute.
Source of information: https://isis.unistra.fr/ + Scopus with search affiliation = (ISIS OR "ingeniérie supramoléculaire*" OR "supramolecular engineering") and affiliation city = Strasbourg

The Institute of Theoretical and Computational Chemistry (IQTC) of the Universidad de Barcelona is integrated by more than 100 researchers, experts in several fields of the Theoretical and Computational Chemistry. The research activity carried out at the IQTC covers methods and computational tools development, application of several techniques of electronic structures and simulation to problems in materials science, the study of reactivity and reaction dynamics in chemical reactions as well as of biological systems and soft-matter. The main goal is to generate synergies between researchers encouraging the interdisciplinary activities that allow to tackle new challenges. Another important goal is to share expertise in handling the computational resources, which are the main tools in this type of research. It employs 33 Principal Investigators, 17 senior researchers, 6 postdocs, 50 PhD students, and 4 administrative and technical staff at the end of 2022. There is no publicly available information on the budget of this institute. We have included this Institute in the comparison because IQCT is a María de Maeztu unit.
Source of information: https://www.iqtc.ub.edu/ + Scopus with search affiliation = (iqtc OR "Teorica i Computacional"" OR "Theoretical and Computational") and affiliation city = Barcelona

The Institute of Molecular Science (ICMol) was founded in 2000 to develop a competitive and high-quality research in materials science using a molecular approach. In fact, ICMol is the sole research center in Spain exclusively focused on the molecular aspects of Nanoscience, with a special emphasis on the study of functional molecules and materials exhibiting useful magnetic, electrical or optical properties. It employs 16 Principal Investigators, 48 senior researchers, 47 postdocs, 98 PhD students, and 36 administrative and technical staff at the end of 2022. There is no publicly available information on the budget of this institute. We have included this Institute in the comparison because ICMol is a María de Maeztu unit.
Source of information: https://icmol.es/ + Scopus with search affiliation = (icmol OR "Ciencia Molecular" OR "Molecular Science") and affiliation city = Valencia

| Institutes | PIs(*) | Senior res.(*) | Postdocs(*) | PhDs(*) | Other(**) | Total(*) | Publications(***) | Top(****) | Citations(*****) | ERC(******) |
|---|---|---|---|---|---|---|---|---|---|---|
| *Stratingh Institute* | *18* | *-* | *30* | *98* | *8* | *154* | *645 (4.4)* | *155 (24%)* | *13586 (21.1)* | *2* |
| *Hylleraas Centre* | *7* | *19* | *9* | *32* | *7* | *74* | *269 (4.0)* | *21(8%)* | *3085 (11.5)* | *1* |
| *ISIS Strasbourg* | *18* | *23* | *49* | *93* | *8* | *191* | *540 (3.0)* | *85 (16%)* | *9563 (17.7)* | *2* |
| *IQTC (Univ. Barcelona)* | *33* | *17* | *6* | *50* | *4* | *110* | *421 (4.0)* | *38 (11%)* | *5967 (14.2)* | *3* |
| *ICMol (Univ. Valencia)* | *16* | *48* | *47* | *98* | *36* | *245* | *489 (2.3)* | *57 (12%)* | *13798 (28.2)* | *3* |
| *IQCC(*******)* | *14* | *5* | *20* | *62* | *4* | *105* | *395 (3.9)* | *73 (19%)* | *6816 (17.3)* | *3* |

*(*) Number of people at 31st December 2022 according to the source. PIs = principal investigators. Senior res. = Senior researchers.*
*(**) Secretaries, research managers, lab technicians, scientific coordinators…*
*(***) Publications in the 2018-22 period. In parenthesis, publications per researchers (PIs+senior researcher+postdocs) (data from Scopus).*
*(****) Publications of the 2018-22 period in Nature, Science, Nature Chem., Nature Commun., Chem, J. Am. Chem. Soc., Angew. Chem., Chem. Sci. (data from Scopus).*
*(*****) Citations to the publications of the 2018-22 period on 1st May 2023. In parenthesis, citations per paper (data from Scopus).*
*(******) Number of ERC StG, CoG, AdG, SyG and Proof of Concept awarded in the 2018-22 period.*
*(*******) Data from Scopus with search affiliation =("computacional i catàlisi" OR "computational and catalysis" OR "computacional y catalisis") AND affiliation city = Girona. The real number of published papers is 470 papers but we use here 395 that result from this Scopus search to make the comparison more reliable.*

As to the non-competitive budget provided every year by the university or by the national or regional governments, the IQCC receives about 30.000 € from the UdG. We can only compare this funding with the 1.275.000 € provided by the Research Council of Norway every year to the Hylleraas Centre for Quantum Molecular Sciences. Certainly, the two quantities differ by a great amount. The funding of the IQCC comes almost exclusively from competitive sources. As to the number of researchers, the IQCC has a similar number to that of the IQTC. In both Institutes, the number are larger than that in the Hylleraas Centre for Quantum Molecular Sciences but smaller than that of the rest of the Institutes. In absolute values, the scientific production of the IQCC is almost identical to that of the IQTC and it is larger than that of the Hylleraas Centre for Quantum Molecular Sciences but smaller than that of the rest. In relative terms (publications per researcher), the IQCC with 3.9 papers per researcher in the 2018-22 period has a similar number than the rest, except for the ICMol that has 2.3 papers per researcher. Most importantly, the quality of the research output of the IQCC is similar to that of the Stratingh institute and the ISIS Strasbourg and considerably above that of the IQTC, ICMol, and the Hylleraas Centre for Quantum Molecular Sciences. The number of citations per published paper in the IQCC is similar to that of the ISIS Strasbourg but larger than that of the IQTC and Hylleraas Centre for Quantum Molecular Sciences and smaller than that of the Stratingh institute and the ICMol. Finally, an important aspect is the number of ERC Starting Grants, Consolidator Grants, Advanced Grants, Synergy Grants and Proof of Concept awarded to members of each institution. As can be seen in the Table, IQCC together with IQTC and ICMol leads this classification.

# Strategic Aims

Education, research, and societal impact are the three key focal points of the IQCC, through which we aim to achieve our mission. The long-term goal of the IQCC is to grow further and stronger, with more opportunities for training young researchers, and receiving recognition for it from the Catalan/Spanish government (Seal of Excellence, María de Maeztu) and the European Commission.

## Education

One of the main objectives of the IQCC is to actively participate in the scientific education and training of young people, starting at secondary school level and working right through to post-doctoral studies. We aim to provide our students and young researchers with the best possible environment to develop their talent and prepare themselves for careers related with science in academia and industry.

The focus of the training is put on the master's and PhD studies. For these activities, we have two 'baseline' actions that provide the basis for the training:

1. Ensure that both master's and PhD research students are provided with suitable space and adequate equipment to permit them to undertake their research activity in satisfactory conditions.
2. Facilitate the access of students with disabilities to master's and doctorate programs in accordance with their possibilities.

## Master in Advanced Catalysis and Molecular Modelling (MACMoM)

Training at the master level is done through the institute's organized and managed master, MACMoM. MACMoM has been active since 2013 and has the aim of directing the students towards more sustainable, efficient and economical catalytic methodologies. Its three pillars are:

- International orientation by being taught entirely in English.
- Orientation to both academic research and industry by providing opportunities to do the Master's Thesis at the institute research teams or at industrial placements.
- Training through a combination of an experimental and theoretical approach to catalysis.

### *MACMoM Related Objectives*

- To consolidate MACMoM by maintaining excellence in teaching and attracting a high number of local (UdG) and external (national and international) students from Chemistry and related disciplines.
- To strengthen the industrial orientation of MACMoM as a way to attract students and as an incentive for technology transfer from the institute.
- To achieve recognition by the UdG of the strategic interests of MACMoM for the university.
- To establish an Erasmus Mundus Master program based on MACMoM.

### *MACMoM Strategic Actions*

1. Identify and contact potential foreign partners to create an Erasmus Mundus Master and work with the OITT to obtain the qualification.
2. Support the implementation of the dual degree in Chemistry and Physics promoted by the Chemistry Department, and similar dual degrees, as a way to attract excellent students. Recognize that improving the Bachelor Degrees of the Faculty is beneficial for the institute and the MACMoM.
3. Support the creation of possible degrees related to Chemistry such as a degree in Materials Science or a degree in Nanoscience and Nanotechnology.
4. Disseminate IQCC research among students from the UdG Faculty of Science (Science Slam) to involve them early on in research (pràctiques en empresa, TFG), and carry out other publicity measures inside and outside the UdG such as participation in Erasmus exchange programs.
5. Promote research grants from IQCC groups to support the students during their Master's Thesis.
6. Increase internationalization by promoting dual degree programs and student-exchange agreements with international universities, as well as recognition from foreign financing agencies.
7. Strengthen MACMoM industrial orientation by establishing new agreements with chemical companies for industrial placements.
8. Consider the option to restructure the master to make it more attractive to potential students.

## Doctoral training

Doctoral training is one of the strengths of the IQCC, as shown by the number of defended PhD thesis and the positions reached by the alumni in academia and industry. The main strengths of our scientific doctoral training are: (i) international top-level research that provides excellent scientific skills, together with the opportunity to interact with world leaders in their field; (ii) high internationalization by promoting placements at international top research centers as a way to reach International Doctorates, and by establishing joint doctorate agreements.

### *Doctoral training Objectives*

- Consolidate our excellent scientific training.
- Improve the training of transversal skills as a way to increase employability towards industry and academia.

### *Doctoral training strategic actions*

1. Establish a Training Committee formed by thesis directors and students that will be in charge of monitoring the following measures, to express the IQCC commitment to improve doctoral training.
2. Set up a Personal Career Development Plan for every PhD student together with the necessary monitoring procedures, and evaluate the possibility of setting up a mentorship plan.

3. Establish a Code of Good Practice in Training for the student and the thesis supervisor and director(s). The code should provide guidelines for supervision and emphasize active participation of the student in interpretation of the results and paper writing.
4. Organize soft and scientific skills transfer courses that complement the ones from the UdG Doctorate School, and achieve recognition of these courses by the Doctorate School.
5. Promote joint industrial doctorates and industrial placements for academically oriented doctorates, using the MACMoM as a platform.
6. Promote international PhD student mobility in all aspects to achieve International Doctorates. This includes attendance/participation in conferences and winter/summer schools, research stays, industrial placements, as well as visits of external graduate students and post-docs to the institute.
7. Establish a Welcome Plan for new PhD students to facilitate their integration in the institute.
8. Establish forums at all possible levels for research presentation by the students (from institute to research team).
9. Promote agreements with international partners to carry out joint doctorate degrees.
10. Contribute as much as possible to obtaining the mention of excellence in the upcoming AQU accreditation of the PhD program in Chemistry.
11. Foster the visits of PhD candidates to foreign labs to get the international mention to their PhD title.

## Research

The IQCC is a university research institute of the UdG. As such, research and education are its two missions and are naturally and inextricably intertwined. IQCC operates internationally and uses synergistic cooperation between theoretical and experimental teams to address scientific global challenges ligated to chemical sciences, expanding the limits of knowledge and providing innovative solutions. Research at the IQCC aims at contributing to the sustainability of our society. We believe that in order for chemistry to support sustainability and guarantee that the necessary chemical products and processes are waste-free, useful, and safe for both people and the environment, there is a need for a triple focus on efficiency, safety, and circularity.

Our vision is that chemistry and catalysis are some of the most effective transformative tools for reaching sustainable societies. With this consideration in mind, the main scientific objective of the unit is the development of new approaches in catalysis to reach the goals of Responsible Consumption and Production, Good Health and Well-Being, and Affordable and Clean Energy.

The research lines of the IQCC in the coming years will be devoted to sustainable chemistry as a way to offer a pathway to reducing the environmental footprint of chemical processes and products, safeguarding human health, conserving resources, and addressing pressing global challenges such as climate change and pollution. By integrating sustainability into chemical practices, we aim to create a more resilient and harmonious relationship between human activities and the natural world.

### *Current main research lines of the IQCC*

Research efforts are concentrated on three main lines of action;

- Homogeneous catalysis aiming at the development of more sustainable chemical synthesis methods, based on earth-abundant metals, valorizing available feedstocks.
- Enzymatic and supramolecular catalysis (chemistry at confined spaces). The aim is the design of enzymes and small-molecule systems for studying and taking advantage of the sustainable features of enzymatic systems and the singular chemical properties of confined spaces.
- The development of computational chemistry tools necessary to bridge the gap between theory and experiment and increase the success in providing ideas and solutions to sustainable-related chemical problems.

### *Strategic research lines for the coming years*

In the coming three years, the strategic research lines of the IQCC that will be pursued are the following:

- Evolution towards more sustainable production methods via establishing homogeneous catalysis methodologies with novel or alternative selectivities. Different lines include the following:
    - Catalytic technologies based in earth abundant metal.

    - Catalysis in non-conventional organic solvents (water, deep eutectic solvents, micelles….).
    - Valorization of feedstocks via selective C–H functionalization.
    - High added-value materials via selective C–C cyclization reactions.
    - Single-step rapid build-up of chemical complexity.
    - Small molecule activation; $CO_2$, $N_2O$, $N_2$, $H_2O$, $O_2$.
    - Catalysis for polymer upgrading, recycling, and degradation.

- Enzymatic catalysis enabled by computational design.
    - Evolution via remote mutations.
    - Alternative mechanisms in Fe-dependent oxygenases.
    - Plastic degrading enzymes.
    - Biocatalytic platforms for biosynthesis and solar fuel generation.

- Catalysis in confined spaces
    - Catalysis in supramolecular vessels.
    - Enzymatic catalysis.

- New generation of solar cells
    - Design of improved components for new generation of solar cells via supramolecular catalysis.
    - Leveraging Singlet Fission and Triplet-Triplet Annihilation for the design of the next generation of organic solar cells.

The IQCC is worldwide recognized as a center of excellence in the development of new computational tools for chemical bonding analysis, calculation of molecular properties, and new approaches to density functional theory. Moreover, with the surge of artificial intelligence, it is also strategic that our Institute becomes known for the development and implementation of machine learning techniques. This policy is in line with the UdG 2030 strategic plan "*sum of intelligences*" of the University of Girona, which is based on a series of actions in which the natural, artificial, and collective intelligences are showcased, to offer comprehensive learning, assured emerging talent, and social impact.

- Development of new approaches in computational chemistry necessary to bridge the gap between theory and experiment
    - Implementation of machine learning methods as general tool to address experimental problems;
        - In nanomaterials for energy related applications.
        - In homogeneous catalysis design.
        - In enzyme design.
        - In smart bio- and molecular materials design.
    - Development of new computational tools;
        - To rationalize and design smart bio- and molecular materials
        - To determine molecular properties such as non-linear optical properties.
        - To analyze chemical bonding: energy decomposition analysis, oxidation states, electron delocalization, aromaticity, etc.
        - To improve current density functional methods.

## Open Science, FAIR Data

The communication of science nowadays involves sharing papers (Open Access), research data (Open Data), software (Open Source), recognition, evaluation and peer review, reproducibility and other aspects of Open Science. The IQCC strongly supports this sharing, through education (Open Science course), our own data server for computational results (IoChem-BD), the server developed by CSUC for experimental data (CORA.RDR), and following closely the international developments to implement these at the local level.

*Open Science Objectives*

- Consolidate our infrastructure for hosting Open Data from computational chemistry.
- Invest in infrastructure for hosting Open Data from experimental chemistry, through Electronic Lab Notebooks.
- Improve the training of Open Science skills as a way to increase reproducibility and reach the standards requested by European Projects.

*Open Science strategic actions*

1. Establish an Open Science Committee formed by experts in the field that will be in charge of monitoring the following measures, to express the IQCC commitment to improve the use of Open Science practices.
2. Establish a Code of Good Practice in Open Science for the researchers.
3. Organize Open Science courses that complement the ones from the UdG Doctorate School, and achieve recognition of these courses by the Doctorate School.
4. Include the Open Science infrastructure and Code of Good Practice into the Welcome Plan for new researchers to facilitate their integration in the institute.
5. Promote agreements with (inter)national partners to carry out joint efforts in Open Science.

## Societal Impact

The societal impact of the IQCC involves the collaboration with industry in research projects, technology transfer through setting up of spin-off companies and obtaining patents, science communication, and in collaboration with the C4D unit performing outreach to the general public and primary/secondary schools.

## Collaboration with industry

There has been a steady increase in collaborative projects with industry, in particular within the field of enzyme design and biocatalysis and with several industrial doctorates.

*Objectives Collaboration with industry*

For the next three-year period, the objectives for collaboration with industry are the following:

- Consolidate the existing collaborative projects with industry.
- Identify possible partners in industry for which the IQCC technology would be useful.

*Collaboration with industry Actions*

1. Consolidation of the IQCC-Industry annual event, which was started in 2020, as a platform for networking with industry, and creating links to IQCC research.
2. Consolidation and extension of the number of industry partners for hosting MACMoM students in internships.
3. Increase the number of joint Industry-Academia PhDs.
4. Pursue EIC Pathfinder applications.

## Technology transfer

The research developed in the IQCC has led to the following main technology transfer achievements: (i) discovery of active sustainable catalysts with potential broad applicability in various commercial fields; (ii) development of more accurate computational tools for describing experimental systems of interest; (iii) development of methodologies for the purification of higher fullerenes and endohedral metallofullerenes (EMFs); (iv) development of methodologies for the regioselective functionalization of fullerenes and EMFs; (v) development of methodologies for rational design of enzymes; (vi) development of methodologies to generate open fullerenes for the application in solar cells; (vii) incorporation of the DiMoCat group in the Catalan XRE4S network energy for society.

*Objectives Technology transfer*

For the next three-year period, the objectives for technology transfer are the following:

- maintain all current science actions and establish new activities to build up a strong local and international reputation.

- increase the technology transfer activities of IQCC and expand the service portfolio for the already constituted Spin-off company GIOXCAT, including consulting in catalysis, O-isotope labelling of organic compounds (reagents and final products), purification of higher fullerenes and EMF, and regioselective functionalization of fullerenes and EMF.
- study the feasibility of bringing the developed computational technologies into pre-commercial stages.
- generate a new spin-off.

*Technology transfer Actions*

1. translate current research accomplishments in patents and identify companies that will be interested in licensing them.
2. identify and apply for funding calls, specially within EU-research frames for directed synergistic applied-fundamental research.
3. development of knowledge transfer action plan (KTAP) for the commercial availability of a portfolio of new sustainable catalysts and new computational tools with different applications.
4. incorporation of more IQCC groups to the Catalan networks that promote the technology transfer and valorization of energy technologies to industry and society.

## Science communication

The IQCC organizes since 1993 the series of biannual Girona Seminars, redesigned in 2015 to align with the strategic objectives of the Institute. Since then, the main topic has been Predictive Catalysis with editions focusing on transition-metal chemistry (2016, 2018), biocatalysis (2022) and for the next edition supramolecular chemistry (2024). Furthermore, through the Communications committee it organizes quarterly IQCC Forums, and an annual Science Slam to attract second/third year Chemistry students to join the IQCC research groups, IQCC Challenges – Live Talks and open IQCC doors.

*Objectives Science communication*

For the next three-year period, the objectives for science communication are the following:

- Maintain all current science communication actions and establish new activities to build up a strong local and international reputation.
- Consolidate the Communications committee that promotes science dissemination and communication.

*Science Communication Actions*

1. The IQCC will organize the biannual Girona Seminar to showcase the most significant results of the IQCC and at the same time invite the principal investigators in the field to share their knowledge and recent studies. This exchange of information and knowledge will improve the research capabilities of the IQCC (and Catalan/Spanish research area) and lead to a learning experience for young researchers in the state-of-the-art of the field. It also fosters collaboration among participants, which may be supplemented through mobility programs available through national and European networks such as COST Actions or ITN projects.
2. The IQCC will organize the IQCC Forum to provide the opportunity for young (and more advanced) researchers to present their work to a wide audience. This training opportunity for science communication will lead to better knowledge of the work that is being performed in all the different research groups of the institute, and enables the researchers to enhance their presentation skills and communicate their exciting new findings to peer scientists.
3. The IQCC will organize additional one-time conferences, symposia at national and regional meetings, and participate in organization of events that are organized by the Catalan Society of Chemistry (SCQ).
4. The website of the IQCC IQCC (http://iqcc.udg.edu) and social networks (Linkedin “IQCC Univ. Girona” and Twitter @IQCCUdG) will be regularly updated with new scientific outputs, and will continue to grow and improve its active connection with stakeholders: from businesses and industries to citizens, from schools to other research groups.

## Collaboration with the C4D unit

The focus of the Unit for Science Culture and Digital Communication (C4D) of the UdG (directed by Dr. Sílvia Simon) is on the promotion of research and study at the crossing points of the fields of communication, science and technology.

*Objectives Science dissemination and outreach*

For the next three-year period, the objectives for science dissemination are the following:

- Maintain all current science actions and establish new activities to build up a strong local and international reputation.

*Outreach activities Actions*

1. Organization of new dissemination activities: The IQCC will be involved in Fairs, Contests, Science Communication Meetings, Public Science workshops, both at a regional and at an international level to build up a strong local and international reputation that can add to the research quality of IQCC's researchers and groups. IQCC strategic objectives related to sustainable production methods through homogeneous catalysis and the importance of converting energy into chemical bonds for the future of our Society will be specially addressed. A summer campus for high-school students will be organized to increase the interest for chemistry and physical sciences in general.
2. Gamification will be used to disseminate the intrinsic components of the main IQCC objectives. Likewise, the understanding of the scientific methodology underlying computational simulations will be promoted using apps for mobile devices, which are more appealing to young students and citizens of all ages.
3. Organization of the European Research Nights coordinated by the IQCC since 2008.
4. Collaboration with the Foundation Institut Jaume Vicens Vives to offer short-term grants to high school students to carry out research stays at IQCC.

# Internationalization

The internationalization is one of the strengths of our institute. The international leadership of IQCC is evidenced by:

1) Success in the ERC-program; Previously to 2018, up to three ERC StG, 1 CoG, and 3 PoC Grants had been granted to IQCC members. These grants originated research lines that have been funded by new ERC Grants in the 2018-2022 period, providing strong credibility for the excellence of their respective research lines;

- ERC-AdvG, Enantioselective C-H Oxidation Guided by Rational Catalyst Design (ECHO-GRACADE), ERC-2019-AdG-883922 was granted to M. Costas (2020-2025).
- ERC-CoG, Fast yet accurate routine rational design of novel enzymes (FASTEN), ERC-2022-CoG-101088032 was granted to S. Osuna (2023-2028).
- ERC-PoC Grant, Computational design of industrial enzymes for green chemistry (GREENZYME), ERC-2022-POC-101112805 was granted to S. Osuna (2023-2025).

2) Participating in and leading International Collaborative Projects from competitive funding:

- COST Action CM1305 (EU-H2020): "ECOSTBio" (2014-2018); M. Swart was the coordinator of the project; M. Costas and A. Company were participants.
- COST Action CA15106 (EU-H2020): "C-H Activation in Organic Synthesis" (2016-2020); X. Ribas and M. Costas were participants.
- International Training Network (EU-H2020): "Non-Noble Metal Catalysis, NoNoMeCat" (2016-2019); M. Costas was one of the eight research leaders, group leader of the oxidation catalysis Work Package.
- Transborder Project (GenCat): "Groupement de Recherche International" network (2015-2018, 2019-2022); A. Pla-Quintana, A. Company, X. Ribas, and M. Costas participate.
- FetOpen Consortium (EU-H2020): "FRINGE" (2019-2023); Ll. Blancafort is leading one of the research lines in multidisciplinary project for new cancer therapies.

- HFSP Grant, "Evolution of conformational and kinetic ensembles during functional transitions, RGP0054/2020 was granted to S. Osuna (2020-2023), together with Dr. Tokuriki (coordinator, U. British Columbia, CAN), Dr. Fraser (U. of California San Francisco, US), Dr. Noji (Tokyo U., JP).
3) Selected international awards received by members of the institute in the 2018-2022 period are EuChemS Lecture Award (S. Osuna, 2021), Marcial Moreno-Mañas Award of the Spanish Society of Chemistry (S. Osuna, 2021), Bioorg. Chem. Award of the Royal Society of Chemistry (M. Garcia, 2021), Fellow RSC (M. Costas, 2020), Cat. National Research Award for Young Talent (S. Osuna, 2019), Honorary Member Polish Chem. Soc. (M. Solà 2019), Member Acad. Europaea, (M. Swart 2019), Young Investigator Award by Lilly and RSEQ (S. Osuna 2019).
4) Members of the institute are Keynote/Plenary speakers at prestigious conferences accessible by invitation. S. Osuna (2022 EuChemS conference., and 2022 Solvay conference., 2020 Gordon Research Conference), M. Costas (Burgenstock conference, 2019), M. Solà (2019 Solvay conference), M. Solà (2022 Gordon Conference).
5) Leading granted outreach projects at the European level; H2020-MSCA-NIGHT-2020 and HORIZON-MSCA-2022-CITIZENS.
6) Very active international research collaborations (63% of papers of IQCC are joint publications with foreign groups).
7) More than 30% of the current IQCC members are from abroad or did the PhD in a foreign Institution.

*Objectives internationalization*

For the next three-year period, the objectives for internalization are the following:

- Maintain all current internationalization actions and establish new activities to improve visibility and to build up a strong international reputation.
- Increase the funding coming from international agencies.
- Increase the number of organized international events.

*Internationalization Actions*

1. Increase the participation in international networks. IQCC should increase its participation in international networks such as the European Joint Doctorate Networks – EJD, Future and Emerging Technologies – FET, and Research and Innovation Staff Exchange - RISE.
2. Promote research seminars held internally at the IQCC by inviting recognized researchers from different scientific or geographical areas. Give priority to invitations to young women researchers whom we think might be interested in becoming part of the IQCC through an ICREA contract.
3. Foster the members of IQCC's relations with the international scientific community (organization of conferences, attendance at conferences, ...).
4. Promote the visits of IQCC PhD candidates to foreign labs and the visits of foreign researchers to the IQCC.
5. Increase the number of members of the IQCC with ERC and MSCA grants.

# Human Capital

The IQCC recruits annually new BSc/MSc students, PhD students, and postdocs, most often through competitive fellowships from the Spanish/Catalan government or European Commission. In 2015, the IQCC started a new tradition of organizing an annual Science Slam for attracting BSc students, in which the PIs of the institute give a 2-minute overview of their research. No such centralized program for attraction of new talent is yet in place for the MSc/PhD students, postdocs or staff.

## General talent attraction and retention

The UdG received the HR Excellence in Research award in 2020, making the IQCC more attractive to national and international researchers.

*General objectives for talent attraction and retention*

For the next three-year period, the general objectives for talent attraction and retention are the following:

- Get more funding for attracting new early-stage researchers and postdocs to the IQCC research groups.

*General Actions for talent attraction and retention*

1. Pursue the María de Maeztu seal of excellence as a way to incorporate new PhD candidates and postdocs and facilitate the retention of the researcher manager and technicians.
2. Update the IQCC website with a "Join Us" section where all offers and calls will be posted.
3. Participate as much as possible in all initiatives concerning talent (excellence) recruitment, like those organized by Caixa de Catalunya or similar initiatives.
4. Set up an IQCC Alumni organization and use it to have good candidates for the positions offered.
5. Taking external constraints into account, pursue a harmonious growth of the experimental and theoretical parts and the three groups that make up the IQCC.
6. Support and provide assistance to all researchers who join IQCC. Welcome them when they arrive and help them settle in. Develop a welcoming plan and networking IQCC activities.

## BSc/MSc students

The IQCC provides a clear education career path, going from BSc to MSc and continues towards the PhD level. The smooth transition and flow of students along this training path requires a constant ingress of new young talent.

*Objectives BSc/MSc students*

For the next three-year period, the objectives for BSc/MSc students are the following:

- Consolidate the annual Science Slam for attracting new BSc students to the IQCC research groups.

*BSc/MSc students Actions*

1. Consolidation of the annual Summer Fellowships for BSc students to enter the world of scientific research through summer projects.
2. Set up an annual recruitment event for prospective Master students to join the MACMoM program.

## PhD students

The PhD program in Chemistry at the UdG has been accredited by the Catalan Agency for Quality promotion and assurance, to which the PhD theses developed at the IQCC have contributed greatly.

*Objectives PhD students*

- Consolidate the number of PhD students, and maintain the high level of scientific research that is described in their PhD theses.

*PhD students Actions*

1. Promote agreements with international partners to carry out joint doctorate degrees.
2. Promote formal agreements with international partners to carry out jointly supervised degrees.
3. Set up annual recruitment event at the IQCC level for PhD fellowships provided through research projects.
4. Set up annual pre-screening events at the IQCC level for prospective PhD students to apply for competitive fellowships.
5. PhD positions, when available, will be posted on the IQCC website in the "Join Us" section.
6. Allow PhDs to attend at least one international conference per year.

## Postdocs

The normal way of entering the IQCC at the postdoc level will be either the two-year Juan de la Cierva, Marie Skłodowska-Curie Research Fellowships, or equivalent program. In addition, the application for three-year Beatriu de Pinós and La Caixa calls (Retaining) will be promoted. Young doctor researchers showing capacity of leading an independent research line and attract funding could be promoted to PI.

*Objectives Postdocs*

- Consolidate the number of postdocs, and maintain the high level of scientific research that is described in their scientific publications.
- Foster the academic career of IQCC postdocs within the IQCC and outside.

*Postdocs Actions*

1. Set up annual recruitment event at the IQCC level for postdoc fellowships provided through research projects.
2. Set up annual pre-screening events at the IQCC level for prospective postdocs to apply for competitive fellowships.
3. Postdoctoral positions and postdoctoral fellowship calls will be posted on the IQCC website.
4. Promote the research independence of postdocs as a way to facilitate their academic career.
5. Establish a Career Development Plan for non-permanent researchers (Postdocs, Emerging Leaders). Including expectations and fulfillment statements and list of commitments.
6. Establish a Career Evaluation Committee that will periodically (annually) evaluate the performance of non-permanent researchers.
7. Create an Emergent leader position within the IQCC awarded by the Career Evaluation Committee. An Emerging leader will be the prior step before being promoted to Principal Investigator.
8. Organize annual polls where the researchers can provide opinions on whether the IQCC has satisfied its commitments.

## Support staff

The IQCC research groups have been providing funds from research projects for contracting a computational technician (since 2005), a project manager (since 2008), and an experimental technician (since 2011). These positions are therefore structural and strategic for the UdG, and should be provided by the UdG, and not come at the expense of research projects.

*Objectives Support staff*

- Consolidation of the structural positions of the IQCC technicians and project manager, with funds from the UdG or from Spanish and Catalan calls.

*Support staff Actions*

1. Hold meetings with UdG Rectorate for convincing them that the staff assigned to the IQCC should be the one needed according to the volume of work and resources that the IQCC generates. Ask for the consolidation of the IQCC technicians and project manager. This staff is essential for IQCC's activity and lack of these positions may seriously compromise current activity and future potential.
2. Claim the need to increase the number of permanent administrative staff associated with IQCC by hiring two full-time administrators and asking for additional administrative support to be maintained.

## Staff

The normal way of entering as a permanent research at the IQCC is through a Ramón y Cajal (RyC) contract or with an ICREA senior contract.

*Objectives staff*

- Incorporate new permanent researchers in the IQCC.
- Provide necessary means to perform research to all permanent researchers in the IQCC as a way to retain talent.
- Provide permanent positions for Starting Grant and Consolidator Grant researchers and Ramón y Cajal researchers with I3 accreditation.

*Staff Actions*

1. Modify the policy for attracting ICREA Senior researchers and give the highest priority to all those endorsed by an active principal investigator. Make the process as transparent as possible.

2. Support and promote the consolidation of Starting Grant and Consolidator Grant researchers and Ramón y Cajal researchers with I3 accreditation, with permanent positions within the IQCC and Department of Chemistry.
3. Convince the UdG Rectorate of the need to hire RyC researchers that want to join the IQCC.
4. Provide maximum assistance so that IQCC-trained doctors who want to can reintegrate into the institute after doing a post-doc abroad.
5. Accomplishments like Starting Grants, Consolidator Grants, and similar outcomes will lead indeed to consider researchers as quasi-permanent (if they are not already permanent). The IQCC will support and promote the creation of permanent positions within the Department of Chemistry and University of Girona for researchers fulfilling the above-mentioned accomplishments.

## Promotion of gender equality

There is growing concern in the EU with regard to the under-representation of women in scientific careers. It has been found that there is considerable wastage of women's skills and knowledge as a result of the disproportionately high levels of women who abandon their scientific careers at all stages. Awareness of this, which is substantiated by extensive statistics, is a first step towards addressing the issue of gender bias.
In the undergraduate studies of Chemistry at the University of Girona more than 50% of students are women. Moreover, a good number of PhD students in the Department of Chemistry are also women. In our particular institute, as an example, in the period 2018-2022, 10 of the 27 theses that were defended were presented by women. However, at staff level, there is still room for improvement. Currently the senior staff of the institute consists of 12 men and 5 women. Notwithstanding, it may be expected that the high percentage of female scientists that are currently at the early stages of their research careers (PhD level) will have the effect of redressing this imbalance in the forthcoming years. Although we believe that the institute is progressing well towards gender parity, measures will be introduced to consolidate this tendency.

*Objectives Promotion of gender equality*

- To boost the participation of women in research, especially after the PhD period as well as in the teaching of courses and seminars, the presentation of conferences both at PhD and post-doctoral stages, and to present their candidacies for chemistry prizes. Encourage advanced female researchers to apply for funding projects at national and international level (Government of Spain, Government of Catalonia, European Commission, etc.) as PIs.
- To encourage the participation of women in management activities, including participation in IQCC advisory and management and external evaluation boards (conference scientific boards, conference organizing committees, editorial boards of scientific journals, etc.).
- To encourage women to opt for inclusion in Government of Spain, of Catalonia and European Commission databases for expert evaluation panels for the evaluation of research proposals, pre-doctoral and post-doctoral fellowships, etc.
- To promote a family-friendly working environment. To improve compatibility of the professional and private lives of women and men, the institute operates a system of flexible working hours. In addition, the institute attempts to always schedule meetings within the regular work timetable.
- To promote an equal female-male balance of invited lecturers at IQCC seminars and at congresses organized by the institute.
- To promote an equal female-male balance of the members serving on evaluation committees (PhD defences, scientific positions, etc.).

# Governance

The main governing body of the institute is the Institute Council that reports to the Research, Transfer, and doctorate delegate Commission of the UdG government Council. The Institute Council is made up of the own academic staff and that of the chemistry department assigned to it for the purposes of research, a representation of the students of the MACMoM master, equivalent to a maximum of 10% of the members of the Institute Council,

and the own administration and services staff. It meets at least once per year. The members of the Institute Council elect the person who has to occupy the position of director (D) of the IQCC.

The director is supported by a Steering Committee (SC) formed by the director, the academic secretary, and three members of the three research groups of the institute proposed by the heads of each research group. The Steering Committee is the advisory body of the institute.

The Board of PI's or Advisory Board (BPIs) is formed by the team leaders of the different research lines of the institute (as of September 2023 there are 15 PI's), one representative of the area of communication of science and the coordinator of the master's board. The competences of this Advisory Board are to have periodic informative and advisory meetings with the Steering Committee.

Furthermore, the Institute has five delegated working committees:

i) The delegated website committee ($DC_W$) is made up of the director, the project manager, a PhD student, the IT technician, one PI, and one representative of the area of communication of science. Their task is to keep the website of the Institute up to date and are responsible for presenting new ideas (such as the quarterly interviews with new members), and implementing ideas put forward by, for example, the SAB or IQCC members or the UdG communication unit.
ii) The delegated computational research committee ($DC_{CR}$) is made up of the PIs (as of September 2023 there are 10 PI's) that perform computational research. Their task is to discuss and decide on strategic planning related to computational research, finances related to the computer clusters and contract of the computational technician.
iii) The delegated cluster committee ($DC_C$) is made up of 7 people: the IT technician, four PI's, one postdoc, and one PhD student. The cluster commission is responsible for aspects of organization, infrastructure, planning, system administration, and user management related to the IQCC's main computing cluster. It also advises $DC_{CR}$ on all aspects related to the compute clusters (organization, infrastructure, planning, system administration, user management) and make proposals for improvements.
iv) The delegated science communications committee ($DC_{SC}$) is made up of three PI's, the head of the Scientific Culture and Digital Communication (C4D) unit, the project manager of the IQCC, and one PhD candidate. The scientific communication committee is responsible for all aspects related to IQCC scientific communication. It organizes scientific communication activities such as the IQCC Forum, where PhD students and postdocs present their latest research, the IQCC Challenges, high school student visits to the IQCC, the Science Slam, the IndustryIQCC Forum, etc. IQCC Forums are planned around Autumn, Christmas, and Easter.
v) The gender and diversity committee ($DC_{GD}$) is made up of three PI's and two PhD candidates. It promotes a balanced representation in terms of gender and diversity in courses, seminars, and conferences, and encourage balanced nominations for awards and staff positions. The committee advises on the implementation of policy for a sustainable and healthy work-life balance, and promote flexible working hours. The committee will provide annual reports with proposals for actions to redress significant imbalances, and monitors the training of researchers and staff for gender and diversity issues.

The IQCC also has administrative and technical support (AS).

The Scientific Advisory Board (SAB) is the body responsible for advising the scientific policy of the IQCC and for evaluating its activities. The SAB meets every 2 years to evaluate the progress of the IQCC and make scientific suggestions. It was implemented in 2014 and has visited the IQCC five times, 2014, 2017, 2019, 2021 and 2023. It is composed of eight members selected among prestigious and accomplished professionals in the field of computational chemistry and catalysis. The board is gender-balanced and has four Spanish members and four European members that are very well acquainted with the Spanish and European research systems.

The Institute of Computational Chemistry and Catalysis has an International Business Council (IBC) to promote the valorization of knowledge, technology transfer, and collaboration with industry. It is made up of the director,

the project manager, and five people working in companies with a recognized prestige in the Institute's research fields.

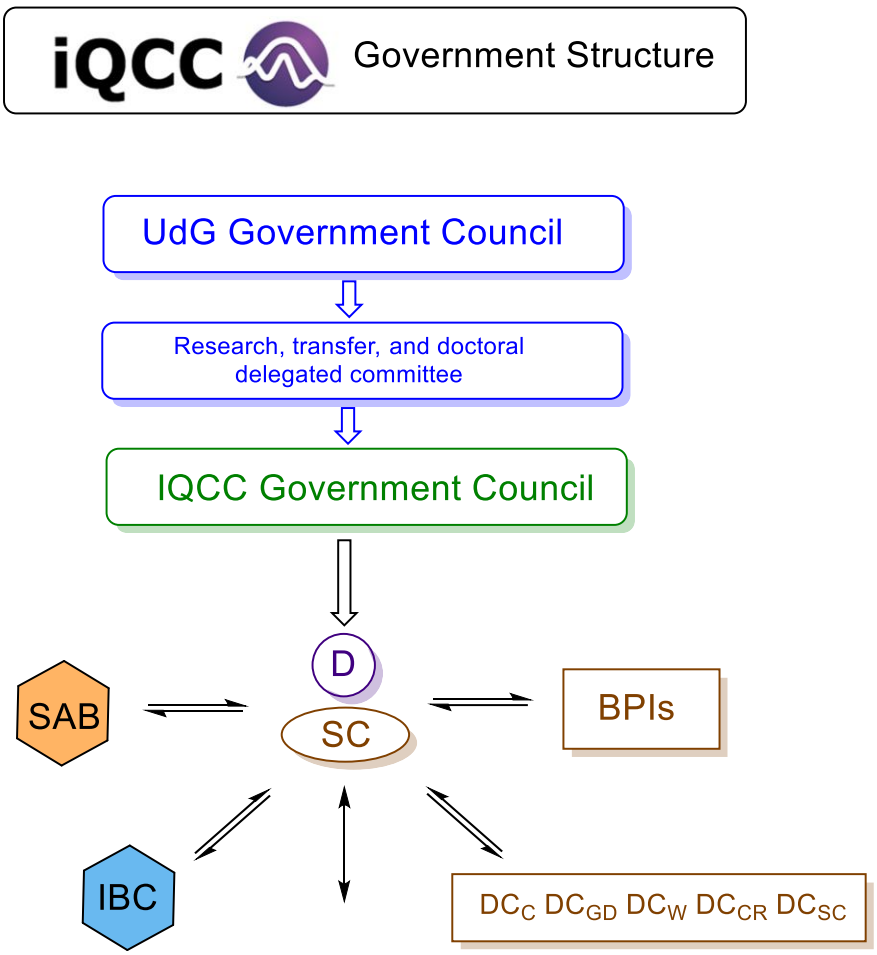
Since 2017 the IQCC organizes an annual survey for receiving feedback on organizational aspects of the institute, what has gone well that year, what has gone wrong, and what could be improved. Furthermore, the input to the IQCC website for keeping it up to date have been automated through online forms for: (i) new publications, (ii) new researchers, (iii) new visitors, (iv) researchers leaving, and v) outreach activities. Since 2019 the IQCC project manager is sending a bimonthly update to the IQCC members to keep them informed about new people, people saying goodbye, new research projects, new publications, new prizes, and other news items.

*Objectives Governance*

- Consolidate the flexible and efficient organization for internal IQCC communications (bimonthly update) and keeping the website up to date.
- Increase the transparency of all decisions taken.

*Governance Actions*

1. Pursue the transformation of the IQCC into a joint Institute in collaboration with some CERCA or CSIC center. Explore other possibilities as well (such as CIQUS, a kind of Promoted University Institute with teaching discounts) with the aim to open new researcher positions.
2. Consolidation of the online forms, and addition of new ones if needed, for efficient internal IQCC procedures.
3. Consolidation of informing IQCC members about administrative procedures, new science policy guidelines, new requirements of Spanish/Catalan governments or European projects.
4. Consolidation of efficient decision-making processes within the three-level step process: first discuss in the Steering Committee, then discuss in length in the Board of PIs, and approve formally at the IQCC Council.
5. Study the possibility of incorporating a research group that does not belong to the Department of Chemistry, such as the Protein Engineering Group or the Differential Equations, Modeling and Applications Group to make the IQCC more interdisciplinary.
6. Consider the possibility to create and launch a delegated experimental research committee ($DC_{ER}$).
7. Argue that the budget received by the University Institutes of the UdG and the teaching discounts from the management should be different depending on the size of the Institute.
8. Provide more autonomy and decision-making capacity to the Committees of the Institute Council: Computational Research Committee, Cluster Committee, Scientific Communication Committee, Webpage Committee, and Gender and Diversity Committee.




## Infrastructure

The experimental labs have all the necessary equipment for organic and inorganic synthesis and experimental characterization. This includes 5 gloveboxes, 13 chromatographs (GC, GC-MS, HPLC, SC-HPLC), 3 UV-vis and FT-IR spectrometers, an electrochemical workstation, 2 multireactors, 2 high-pressure reactors, a polarimeter, a 3D printer, and 2 ion trap mass spectrometer. The unit has two laboratory technicians to handle this equipment.

In addition, the unit owns very singular and advanced mass spectrometry (MS) equipment, namely a high-resolution Bruker micro-QTOF-QII mass spectrometer equipped with a Bruker Cryospray ionization source that enables analyses of samples at very low temperatures (down to -100 ºC). This is one of two instruments of this type operative in Spain. Several researchers from other institutions in Spain, Europe, and America have visited the unit to perform experiments in this particular instrument.

The experimental facilities are completed with the UdG Research Technical Services. This unit offers two 400 MHz and one 300 MHz NMR spectrometer, one X-ray mono-crystal diffractometer (working temperature -173 to +80 °C), one X-ray powder diffractometer, one elemental analysis system, and one MALDI-TOF MS (installed in November 2019).

X-ray absorption spectroscopy (XAS) analyses are carried out in several European synchrotron facilities where beam time is granted upon request and project review, such as SOLEIL (Paris), ELETRA (Trieste), ESRF (Grenoble), ALBA (Barcelona) or DIAMOND (London). Other specialized equipment is accessible via collaborations with research groups in Europe and the US. In the last years, we have had access to resonance Raman equipment (W. Browne, U. of Groningen); spectrofluorimetry equipment (P. Ballester, ICIQ); a single-axis

diffractometer (D. Maspoch, ICN2); EPR equipment (C. Duboc Toia, CEA Grenoble and Alex Guo, Carneggie Mellon U.), IR-MS (J. Roithova, Raboud U.), and Mossbauer spectroscopy equipment (A. Guo, CMU, and S. Ye, MPI Mulheim).

As to the computational facilities, the unit has a CPU cluster with 70 nodes with a dual processor and a total of 1760 cores, a GPU cluster of 22 nodes with a total of 176 GPU and a GPU mini-cluster for testing. These facilities allow IQCC researchers to carry out most of the calculations in-house. The clusters are managed by an informatics technician. For the most demanding calculations, the unit has access to the large-scale facility of the Consortium of University Services of Catalonia (3 M hours in 2022 on a pay-per-use basis) and the nodes of the Spanish Supercomputing Network, which are granted for free on a project basis. We have had 49 projects corresponding to 23.65 M hours (2018-2022 period).

*Objectives Infrastructure*

- Increase the research equipment readily available to IQCC members
- Solve the problems related to the local computational clusters.

*Governance Actions*

1. Facilitate the setup of the new data processing center (CPD) of the UdG.
2. Make a list of research equipment needed by IQCC researchers but not available yet.
3. Apply to all possible infrastructure calls to get financial support for new research equipment.

## Housing

Regarding the space, the IQCC occupies around 550 m² of laboratory and 600 m² of office space distributed in a scattered manner between the Faculty of Sciences (in different buildings and corridors) and the Science and Technology Park (Casademont and Monturiol buildings). The same goes for the infrastructure, which is also dispersed in different spaces.

*Objectives Governance*

- To be hosted in a new IQCC or Chemistry Department building.

*Governance Actions*

1. Convince the UdG Rectorate of the need to have all the IQCC research groups in the same building.
2. Demand more space for offices and research laboratories at the IQCC as a necessity for the Institute to improve its quality.