

Strategic Plan IQCC 2027-2031



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Preamble

The fourth 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 was approved by the institute Council for the period 2005-07 on the 11th March, 2005. There was a second Strategic Plan of the IQCC for the period 2015-2018 that was approved on the 10th June, 2015, and a third Strategic Plan of the IQCC for the period 2024-2026 that was approved on the 25th October, 2023. The current Strategic Plan must mark the lines of action mainly for the next five years, although in some cases the proposed actions can be extended for several more years.

This Strategic Plan marks a transition to a new stage in the evolution of the institute, driven by our ambition to become a CERCA institute. More than two years ago, the former Director of IQCC, Prof. Miquel Solà, initiated discussions with the Catalan Government to explore the possibility of transforming IQCC into a Generalitat de Catalunya research centre, i.e., a CERCA institute. In March 2025, I assumed the role of Director of the institute with the primary objective of leading this transformation and securing CERCA accreditation.

The Strategic Plan 2027–2031 outlines the roadmap for this transition, which is formally initiated with the CERCA evaluation scheduled for the end of 2026. It defines the strategic actions that will guide the institute through this process and position IQCC for its next stage of growth and excellence.

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 for this Strategic Plan were collected by Dr. Teresa Corona when writing the María de Maeztu 2026 application and the CERCA self-evaluation in summer 2026.

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 five years. 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 postdocs 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.

Xavi Ribas
Director

Introduction

In April 2023, the Institute of Computational Chemistry and Catalysis (IQCC) celebrated its 30th anniversary. Having grown from a small team of researchers, it now comprises three consolidated research groups, all of which received official recognition from the Generalitat de Catalunya in mid-2026. At the end of the 2025-26 academic year (July 2026), the institute consisted of 118 researchers (7 full professors, 9 associate professors, 3 ICREA Senior researchers, 2 Ramón y Cajal researchers, 3 ex-professors, 22 postdocs, 72 PhD students) and 7 support staff (1 research manager, 2 technicians, 4 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 has produced a total of 92 PhD theses. Researchers are grouped into three main research groups, all of which are recognized and funded by the Government of Catalonia in its 2025 consolidated group call (SGR-Cat 2025): 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 7 principal investigators, and the Theoretical Chemistry of Biosystems Group (TCBioSys) with 5 principal investigators. On average, during the period 2022-2025, the Institute has received an annual funding of 3.5 M€, most of which comes from competitive European or National Plan calls. The productivity of the IQCC is supported by the publication of 464 articles during the period 2022-2025, which have received more than 6200 citations. Some of these articles have been published in journals such as Science (3), Nature Chem. (5), Nature Synth. (3), Nature Commun. (5), Nature Catal. (6), Chem (1), JACS (31), ACIE (23), Chem. Sci. (19), ACR (1), etc. In the same period, 39 doctoral theses have been defended, 8 of them from 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 European Researchers' Night since 2008 one of its most outstanding activities.



Members of the IQCC, December 2025.

Mission

The IQCC aims to improve society by advancing towards a more circular, 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 improving the sustainability of 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

Sustainable growth is a key priority for Europe, and our vision is that scientific research aimed at transforming production and recycling methods at the molecular level will play a pivotal role in the transition towards a circular economy. Chemical sciences are therefore of strategic importance, enabling more sustainable methods for the production, use, and recycling of the molecules and materials that underpin modern society. They contribute to reducing dependence on scarce resources, developing waste-free and resource-efficient processes, and creating clean energy technologies and recyclable materials.

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, fostering interdisciplinary collaboration to generate transformative scientific advances. Building on these strengths, our vision is for IQCC to become a leading international research institution driving the transition towards a sustainable circular economy.

Values

The institute's research groups conduct pioneering research at the frontiers of knowledge and collaborate closely with leading research centers worldwide. Their scientific achievements are internationally recognized, and they are acknowledged as leaders in a range of fields, including enzyme modelling, bioinspired catalysis, supramolecular chemistry, aromaticity, and computational methodology.

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

The 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 the University of Girona (UdG) on December 31, 1991. On July 6, 1992, the Management Committee of the UdG agreed to initiate the legal procedure for the creation of the Institute of Computational Chemistry (IQCC). Finally, the IQCC 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 IQCC), 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 IQCC, a position he held until 2004. Subsequently, the institute has been directed by **Profs. Miquel Solà (2004-2007; 2023-25), Lluís Blancafort (2007-2015), Marcel Swart (2015-2023) and Xavi Ribas (2025-)**. During the mandate of Prof. Blancafort, the current IQCC was created by joining the groups of the IQCC with the groups of Bioinorganic and Supramolecular Chemistry and Transition Metals in Organic Synthesis, both from the Department of Chemistry at the 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

The IQCC is a research institute that produces internationally recognized cutting-edge research in the fields of theoretical chemistry and homogeneous and enzymatic catalysis. Research at IQCC aims at contributing to the final goal of a circular economy by creating chemical technologies that align with the principles of green chemistry and that implement sustainable methods of production.

To compare the global performance of **IQCC** with other national and international leading institutions, **seven institutions researching in similar fields**, were selected.

The present benchmark is performed using data accessible from the latest Annual or Scientific Reports of these institutions, or the information available on the official websites of the centers. To perform this benchmark the following chemistry institutes were considered:

At national level:

- The **Institute of Materials Structure (IEM)**, part of the Spanish National Research Council (CSIC) in Madrid, is a leading research center focused on the physical and chemical properties of materials, including nanoscience, optics, and surface science. It conducts both fundamental and applied research to advance knowledge in materials science and its technological applications. It is not a María de Maeztu unit.
- The **Center for Research in Biological Chemistry and Molecular Materials (CiQUS)** was created in 2010 by the Governing Council of the University of Santiago de Compostela (USC). It is a singular research center that promotes the advancement of science at the frontier of knowledge in the fields of synthetic chemistry, chemical biology, and functional materials. It became a María de Maeztu unit in 2026.
- The **Institute of Theoretical and Computational Chemistry (IQTUB)** of the Universitat de Barcelona is integrated by more than 90 researchers, experts in several fields of Theoretical and Computational Chemistry. The research activity carried out at the IQTUB covers methods and computational tools development, application of several techniques of electronic structure 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. It is a María de Maeztu unit.
- The **Institute of Chemical Research of Catalonia (ICIQ)** has two main areas of research: Catalysis and Renewable Energy. Its mission is to lead, from the vantage point of molecular science, cross-strategies for solving major social and economic challenges, such as climate change and sustainable supply of energetic and raw materials, thereby contributing to the establishment of a knowledge-based economy and improving quality of life for all. It is a Severo Ochoa center.

At international level:

- The **Otto Hahn Institute (OTI)** in Germany is one of the oldest institutes of the Max Planck Society. It aims at an integral understanding of chemical processes in the Earth system, particularly in the atmosphere and biosphere. Investigations address a wide range of interactions between air, water, soil, life, and climate in the course of Earth history up to today's human-driven epoch, the Anthropocene.
- The **Stratingh Institute for Chemistry** in the Netherlands is a research institute at the Faculty of Science and Engineering of the University of Groningen. The research program is focused on synthesis, catalysis, functional materials, bio-organic chemistry/chemical biology and systems chemistry/complex molecular systems.
- The **Hylleraas Centre** is a Norwegian Centre of Excellence shared equally between the University of Oslo (UiO) and The Arctic University of Norway (UiT). The Hylleraas Centre aims to develop and apply computational methods to understand, interpret, and predict new chemistry, physics, and biology of molecules in complex and extreme environments.

As some of these institutes belong to universities, only on exceptional occasions, economic data or aggregated data from the different laboratories were released. Table I gathers the results of the benchmark, whereas Table II provides the sources of the data.

Table I. Comparison of the global performance of IQCC with other national and international leading institutions (IEM, CIQUS/USC, IQTCUB, ICIQ, OTI, Stratingh, and Hylleraas).

	IQCC	IEM	CIQUS	IQTCUB	ICIQ	OTI	Stratingh	Hylleraas
Year ^a	2025	2024	2024	2024	2024	2022	2025	2024
Input								
Fund raising	3,85	nd ^c	11,5	nd ^c	20,1	6,72	nd ^c	2,52
Staff	125	79	220	140	325	300	143	60,3
PI	16	42	19	42	23	24	17	12
Research areas	3	4	3	3	9b	5	8	5
Publications	117	1209	123	137	148	201	164	83
Active projects	28	40	73	66	92	nd ^c	nd ^c	nd ^c
European ERC projects (SyG, AdG, CoG, StG, PoC)	4	0	14	1	7	nd ^c	nd ^c	nd ^c
PhD Thesis Defended	10	4	22	8	20	7 ^d	36	7
Ratio								
Fund raising/staff x 100	3,25	nd ^c	5,39	nd ^c	6,18	2,24	nd ^c	4,18
Fund raising/PI x10	2,03	nd ^c	6,23	nd ^c	8,74	2,80	nd ^c	2,10
Staff/research areas	37,67	19,75	73,34	45,67	36,11	60,00	17,88	12,06
Fund raising/publications x 100	3,29	nd ^c	9,35	nd ^c	13,58	3,34	nd ^c	3,03
Fund raising/active projects x 10	1,38	nd ^c	1,58	nd ^c	2,18	nd ^c	nd ^c	nd ^c
publications/staff	1,04	1,38	0,56	0,97	0,46	0,67	1,14	1,37
Publications/PI	7,31	2,59	6,47	3,26	6,43	8,38	9,65	6,91
Thesis/PI	0,63	0,10	1,16	0,19	0,87	0,29	2,11	0,58
Thesis/research areas	3,33	0,4	7,33	2,66	2,22	1,4	4,5	1,4

^a Last year from which information can be found.

^b Number of consolidated research groups.

^c nd: no data found.

^d Extracted from the website: <https://www.mpic.de/5536332/Alumni>

Table II. Available Data Sources for the Benchmark Analysis

Centre	Source
CIQUS USC	https://ciqus.usc.gal/sites/default/files/memorias/ciqus_annual_scientific_report_2024.pdf
ICIQ	https://iciq.org/wp-content/uploads/2026/02/D4_Memoria-activitats-ICIQ-2024.pdf
IQTCUB	https://www.iqtc.ub.edu/wp-content/uploads/2025/07/IQTCUB-Report-2024.pdf
IEM	https://www.iem.csic.es/memorias/Memoria_IEM_2024.pdf
OTI	mpic_scientificreport_2023_web_20240119.pdf
Stratingh	https://research.rug.nl/en/organisations/stratingh-institute-for-chemistry/
Hylleras	https://www.mn.uio.no/hylleraas/english/about/annual-reports/hylleraas_2024_web_spreads.pdf

The IQCC has a smaller size in terms of number of employees and number of PIs compared to most national and international centers. However, the benchmark analysis reveals that IQCC ranks amongst the top-performing institutes in terms of per capita publications (1,04), publications per PI (7,31), and we are performing well in the number of PhD theses per PI (0,63). The cost per publication in the IQCC is one of the lowest among the Institutes analyzed. By June 2026, IQCC was the only one among those of Table I that had released the 2025 annual scientific report.

From this brief analysis, it is clear that additional funding would further boost the productivity and excellence of research at IQCC and help the center to become one of the leaders in its discipline on the European scene.

The SWOT analysis

Figure 1 shows the SWOT analysis of the IQCC in summer 2026.

Figure 1. SWOT analysis of the IQCC.

SWOT ANALYSIS		
	Positive	Negative
Internal	Strengths - Strong, well-funded research groups - Strong job placement outcomes - Several ERC grants - Attractive workplace and location - Strong science communication/outreach - Prestigious international conferences organized - High productivity in terms of articles and PhD thesis - Important internationalization in terms of international members and visits to and from the IQCC	Weaknesses - No own building - Limited core funding - Difficulty offering stable and competitive contracts - Weak industry collaboration and tech transfer - Self-employed researchers - Limited number of international staff members
External	Opportunities - Progress toward CERCA Institute - Strong institutional and government support - Access to competitive programs and fellowships - New excellence funding opportunities - Planned UdG Biomedical Park - New Pharmacy degree (2027–28) - Horizon Europe collaborative projects - Access to EU research infrastructures - Synergies with EIC & MSCA programs	Threats - Strong competition from attractive programs and leading institutes - Pressure from UdG to limit permanent staff growth - Low enrollment in MACMoM master - The government allocates money to research increasingly to research centers

From Institute of Computational Chemistry and Catalysis (IQCC) to Institute of Circular and Sustainable Chemistry of Catalonia (IQCS-CAT). Why?

The IQCC is an Institute of research of the UdG, and, therefore, currently the IQCC operates under the umbrella of the UdG, leveraging its infrastructure, academic network, and student body. **University Institutes** excel at exploratory, fundamental research, long-term talent cultivation, and highly interdisciplinary science where student training is a primary goal. This type of organization has several advantages and drawbacks. As the main advantages, we can mention the easy access to master and bachelor students, the access to PhD fellowships (especially those offered by the same UdG), the shared infrastructure & equipment (Technical Research Services), democratic director's election, and academic freedom. As the main drawbacks, we can list the limited core funding offered by the UdG, the difficulties in hiring young and senior researchers (UdG strictly limits the growth of permanent staff that depends on the number of assigned ECTS), the insufficient administrative support, the university bureaucracy, and the restricted access to overhead fees (indirect costs).

The **CERCA Centers** (Centres de Recerca de Catalunya) are a network of independent, high-performance research institutes in Catalonia that operate under a specific institutional and managerial framework promoted by the

Catalan regional government (Generalitat de Catalunya). The CERCA model was created by Andreu Mas-Colell at the beginning of this century to provide Catalan scientific institutes with the flexibility, international competitiveness, and operational freedom typical of independent research centers, while keeping them anchored to the broader academic ecosystem. The CERCA network comprises over 40 top-tier research institutes in Catalonia, including the ICFO (Institute of Photonic Sciences), IRB Barcelona (Institute for Research in Biomedicine), ICN2 (Catalan Institute of Nanoscience and Nanotechnology), BSC-CNS (Barcelona Supercomputing Center), and ICIQ (Institute of Chemical Research of Catalonia), among many others. Some of these institutes form together the **Barcelona Institute of Science and Technology (BIST)**. This type of organization has several advantages and drawbacks. As the main advantages, we can mention higher visibility, high budget, focus on research, streamlined administrative decision-making, flexible human resources (HR) policies, possibility to offer industry-competitive salaries to attract elite researchers, software engineers, and specialized technicians, and easier and more independent negotiation with industrial partners as well as higher intellectual property control. As drawbacks, we have that the center must self-fund its administrative staff, legal teams, facility maintenance, and core equipment, the lack of bachelor, master, and PhD training programs, isolation risks, less academic freedom, and lack of control over the director's appointment.

There is a trend in Catalonia and in different parts of Spain promoted by politicians of increasing the funding of research centers (like CERCA centers) to foster research at the highest level (see for instance: <https://cerca.cat/actualitat/noticies/el-govern-incrementa-en-25-milions-el-financament-als-centres-cerca/>). Such an increase is less often seen at the University level. Although not written in a document, the policies of the government seem to go in the direction of concentrating research and innovation in research centers, while leaving the educational training to Universities.

The model we propose for the new Institute of Circular and Sustainable Chemistry of Catalonia (IQCS-CAT) is parallel to the one currently operating at the Catalan Institute for Water Research (ICRA). ICRA has an agreement with the University of Girona that makes this CERCA center an institution affiliated with the UdG. With this type of agreement, the researchers of the IQCC will assign totally or partially their research to the new IQCS-CAT center, but at the same time they will keep their positions as professors of the Chemistry Department of the UdG. IQCC researchers who assign their research to the IQCS-CAT will maintain the rights and obligations of their original institution (UdG). The IQCS-CAT might provide teaching reductions to some of its researchers, with the amount of reduction being established by the director of the IQCS-CAT. The UdG will grant all IQCS-CAT staff access to its research infrastructure, scientific-technical services, and physical and digital libraries under the same conditions as UdG personnel. This includes campus software licenses, institutional repositories, language and training courses, workshops, seminars, and event participation. The specific terms governing these services will be formally established in a bilateral agreement between the UdG and IQCS-CAT.

Within this model, the IQCS-CAT will have the following advantages:

- access to master and bachelor students
- shared infrastructure & equipment of the UdG (Technical Research Services)
- the increase in the baseline budget (to be negotiated with the Generalitat de Catalunya)
- full access to the overhead fees (indirect costs)
- the flexibility to hire early-career and senior researchers through two avenues: either as faculty members in the Chemistry Department or as research staff at the IQCS-CAT
- fully dedicated and expanded administrative support
- increased visibility for the chemistry research developed at our institute
- flexible human resources policies
- possibility to perform its own research policies (for instance, offer PhD fellowships)
- easier and more independent negotiation with industrial partners and higher intellectual property control.

And the following drawbacks:

- need to self-fund its administrative staff, legal teams, facility maintenance, and core equipment
- loss of some academic freedom
- lack of control over the director's appointment

- loss of access to some PhD fellowships (especially those offered by the same UdG)

In summary, although no scenario is entirely without drawbacks, the case for transitioning from IQCC to IQCS-CAT is strong. The current momentum is exceptionally favorable, supported by the political consensus necessary to bring this project to fruition. We have the approval and support of the government of the UdG (Prof. Josep Calbó, rector), the general director of research of the Generalitat de Catalunya (Dr. Teresa Sanchís), the director of the CERCA centers (Dra. Laia Pallejà), the Minister of Territory, Housing and Ecological Transition, and Government spokesperson (Ms. Sílvia Paneque), and the local authorities from the town hall, the Spanish provincial government, and the Generalitat de Catalunya provincial government.

Transition from IQCC to IQCS-CAT

The transition to IQCS-CAT is envisioned in three steps:

- 1) *Achieving a positive evaluation from CERCA by the end of 2026. If successful, we will negotiate the budget and institute spaces (offices and laboratories) with the Trustees and establish the formal transition date. In the case a reevaluation is needed, the implementation will be delayed accordingly.*
- 2) *Once the transition date is set, the Scientific Director and the Manager will be named and contracted, followed by the gradual and required hiring of the finance administration, technical staff, and HR personnel. This phase is scheduled for 2 years.*
- 3) *The institute's full implementation will require the recruitment of all the necessary administrative and support personnel, including staff in finance, knowledge transfer (KTT), and human resources, as well as technical staff, project managers, and international project coordinators. This phase is scheduled for 2 years.*

The next sections discussing strategic aims, internationalization, and human capital will be followed irrespective of whether we stay as IQCC (university institute) or we transform our Institute into IQCS-CAT (CERCA institute).

Strategic Aims

Education, research, and societal impact are the three key focal points of the IQCC/IQCS-CAT, through which we aim to achieve our mission. The long-term goal of the IQCC/IQCS-CAT 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/IQCS-CAT 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 to science in academia and industry.

The focus of the training is on the master's and PhD studies. For these activities, we have three '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.
3. Ensure that both master's and PhD research students are supervised correctly, with regular meetings with their supervisors.

Master in Advanced Catalysis and Molecular Modelling (MACMoM)

Training at the master level is done through the institute's organized master's program, i.e. 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 pathway and introduce changes in the academic pathway of MACMoM as a way to attract more 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. Disseminate IQCC/IQCS-CAT 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.
3. Promote research grants from IQCC/IQCS-CAT groups to support the students during their Master's Thesis.
4. Increase internationalization by promoting dual degree programs and student-exchange agreements with international universities, as well as recognition from foreign financing agencies.
5. Strengthen MACMoM industrial orientation by establishing new agreements with chemical companies for industrial placements.
6. Consider the option to restructure the master to make it more attractive to potential students.
7. 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.
8. Support the creation of possible degrees related to Chemistry, such as the degree in Pharmacy (expected in 2027/2028) or degrees like Materials Science or Nanoscience and Nanotechnology.

Doctoral training

Doctoral training is one of the strengths of the IQCC/IQCS-CAT, as shown by the number of defended PhD theses 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. Most of the PhD students of IQCC/IQCS-CAT enroll in the PhD program in Chemistry at the UdG. This program has received the mention of excellence recently in the last AQU accreditation.

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/IQCS-CAT commitment to improve doctoral training.

2. Improve the Personal Career Development Plan for every PhD student together with the necessary monitoring procedures.
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 PhD mentoring program to help PhD students to design their professional career.
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. Foster the visits of PhD candidates to foreign labs to get the international mention on their PhD title.

Research

The IQCC is now a university research institute of the UdG. If transformed to IQCS-CAT it will be a CERCA center. In both cases, research and education are its two missions and are naturally and inextricably intertwined. IQCC/IQCS-CAT operates internationally and uses synergistic cooperation between theoretical and experimental teams to address scientific global challenges ligated to sustainability in chemical sciences, expanding the limits of knowledge and providing innovative solutions. Research at the IQCC/IQCS-CAT aims at contributing to the sustainability and circular economy 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 in general and, in particular, 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 blended experimental and theoretical 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/IQCS-CAT in the coming years will be devoted to sustainable and circular 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 and circularity 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/IQCS-CAT

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 in confined spaces). The aim is to design enzymes and supramolecular systems to study and leverage the sustainable features of enzymatic systems and the distinctive 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

Research efforts will be focused on three main lines of action;

L1. Chemoenzymatic degradation.

Plastic materials have been increasingly used over the years, with global production reaching almost 370 million tons in 2020. Some of the most widely used plastics are not biodegradable and accumulate in the environment.

There is an urgent need to develop sustainable plastic degradation technologies in line with the European Green Deal and the EU Circular Economy Action Plan. Some natural enzymes from fungi and other microorganisms can break down complex organic compounds such as plastics. Their biodegradation activities can be improved through enzyme engineering. Polyethylene (PE) and polypropylene (PP), which are the most widely used plastics (50% of total plastic production), are particularly recalcitrant to biodegradation and can take several hundred years to decompose in the environment. At IQCC/IQCS-CAT, we work to depolymerize PE and PP into shorter chains using modified enzymes that facilitate polymer breakdown and enable monomer recovery. In parallel, research is being conducted on the design of new ligninolytic enzymes (lignin processors) as a very promising source of renewable, sustainable, and alternative energy to petroleum.

L2. Sustainable catalyst design to move towards a circular economy.

New technologies that improve the recyclability of synthetic polymers will be one of the main transformative tools towards a circular economy. The development of these sustainable technologies is aligned with the EU Plastics Strategy, a priority for the European Commission, which aims to transform the way plastics are designed, produced, used and recycled in the EU. Ideal transformative tools are new polymers that can be chemically recycled back to their starting monomers, offering a closed-loop approach towards a circular materials economy. With this aim, IQCC/IQCS-CAT is designing catalysts that are capable of producing recyclable polymers and other catalysts that allow the recovery of the starting monomers to restart production.

L3. Advancing solar technology.

The promotion of green and renewable energy is the seventh goal of the UN Member States' 2030 Agenda for Sustainable Development. In addition, the European Green Deal was adopted in 2020 to establish policy initiatives that aim to move towards a sustainable and climate-neutral European Union by 2050. Global warming is putting enormous pressure on the development of carbon-neutral and environmentally responsible technologies for power generation. At IQCC/IQCS-CAT, we explore three different technologies to make solar technology more efficient, environmentally friendly, cost-effective and more sustainable in a circular economy context. Regarding the first technology, fullerenes are regioselectively (poly)functionalized as electron transport materials (ETMs) for perovskite solar cells (PSCs), and nanographenes are designed as hole transport materials (HTMs) in PSCs. The second technology corresponds to organic solar cells (OSCs) that are made up of electron donor and acceptor materials (D-A dyads). Fullerene derivatives are among the most widely used electron acceptors, while donors of various types are used. To improve the power conversion efficiency of OSCs, IQCS-CAT is investigating the use of singlet fission donor (SF) sensitizers, a class of nanographene materials capable of forming two triplet excitons (T_1) from a single absorbed photon. This property has the potential to increase the efficiency of solar cells by up to 200%. The third technology being studied at IQCS-CAT aims to develop sustainable and scalable solar technologies through biocatalysis and photoelectrocatalysis.

Moreover, the IQCC/IQCS-CAT 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. Therefore, the development of new approaches in computational chemistry necessary to bridge the gap between theory and experiment will also be pursued in the IQCC/IQCS-CAT with the following aims:

- 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 compute 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 (Open peer review), reproducibility, ethics, and other aspects of Open Science. The IQCC/IQCS-CAT 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, in collaboration with the NFDI4Chem consortium.
- 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/IQCS-CAT 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. Promote agreements with (inter)national partners like NFDI4Chem to carry out joint efforts in Open Science.

Societal Impact

The societal impact of the IQCC/IQCS-CAT 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 for Collaboration with industry

For the next five-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/IQCS-CAT technology would be useful.

Collaboration with industry Actions

1. Consolidation of the IQCC/IQCS-CAT-Industry annual event, which was started in 2020, as a platform for networking with industry, and creating links to IQCC/IQCS-CAT 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 IQCC/IQCS-CAT has a strong scientific foundation, research areas that are highly aligned with industrial needs, and real examples of technology transfer that demonstrate the model already works. The research developed in the IQCC/IQCS-CAT 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) computational design of molecules showing singlet fission.

We established in 2024 an *International Business Council (IBC)* that every two years evaluates the collaboration with industry and the technology transfer carried out by the IQCC/IQCS-CAT and provides recommendations to follow for the next two years.

Objectives Technology transfer

For the next five-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/IQCS-CAT and expand our service portfolio, including new patents, consulting in catalysis, O-isotope labelling of organic compounds (reagents and final products), purification of higher fullerenes, fullertubes, and EMFs, and regioselective functionalization of fullerenes and EMFs.
- generate a new spin-off.
- study the feasibility of bringing the developed computational technologies into pre-commercial stages.

Technology transfer Actions

1. change the culture of the IQCC/IQCS-CAT and every time we make a discovery, think about its possible application; communication should evolve from describing research outputs to explaining business value.
2. translate current research accomplishments in patents and identify companies that will be interested in licensing them.
3. identify and apply for funding calls, specially within EU-research frames for directed synergistic applied-fundamental research.
4. development of a knowledge transfer action plan (KTAP) for the commercial availability of a portfolio of new sustainable catalysts and new computational tools with different applications.
5. incorporation of more IQCC/IQCS-CAT groups to the Catalan networks that promote the technology transfer and valorization of energy technologies to industry and society.
6. foster incorporation of more professionals with industrial experience to create a unique opportunity to accelerate the development of a more impact-driven and transfer-oriented culture.
7. hire a manager to foster technology transfer at IQCC/IQCS-CAT and take care of all these actions.

Science communication

The IQCC/IQCS-CAT 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), supramolecular chemistry (2024), and Synthesis and functionalization of cyclic compounds (2026). Furthermore, through the Communications committee it organizes quarterly IQCC/IQCS-CAT Forums, and an annual Science Slam to attract second/third year Chemistry students to join the IQCC/IQCS-CAT research groups, IQCC/IQCS-CAT Challenges – Live Talks and open IQCC/IQCS-CAT doors.

Objectives Science communication

For the next five-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/IQCS-CAT will organize the biannual Girona Seminar international conference to showcase the most significant results of the IQCC/IQCS-CAT and at the same time invite the international leaders in the field to share their knowledge and recent studies. This exchange of information and knowledge will improve the research capabilities of the IQCC/IQCS-CAT 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 MSCA-DN projects.
2. During the Girona Seminar, the IQCC/IQCS-CAT will organize the IQCC/IQCS-CAT Young Researcher Symposium 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 enable the researchers to enhance their presentation skills and communicate their exciting new findings to peer scientists.
3. The IQCC/IQCS-CAT will organize additional one-time conferences, symposia at national and regional meetings, and participate in the organization of events that are organized by the Catalan Society of Chemistry (SCQ).
4. The website of the IQCC/IQCS-CAT (<http://iqcc.udg.edu>) and social networks (Linkedin "IQCC Univ. Girona") 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 five-year period, the objectives for science dissemination are the following:

- Ensure that knowledge is effectively transferred to society as a key of our institute responsibility.
- Maintain all current scientific communications 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/IQCS-CAT 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/IQCS-CAT's researchers and groups. IQCC/IQCS-CAT strategic objectives related to circular chemistry and 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/IQCS-CAT 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 Researchers' Night coordinated by the IQCC/IQCS-CAT 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/IQCS-CAT.
5. Launch an IQCC/IQCS-CAT podcast aimed at bridging the gap between cutting-edge research and the general public.

Internationalization

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

1) Success in the ERC-program; Previously to 2022, up to three ERC StG, 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 2022-2025 period, providing strong credibility for the excellence of their respective research lines;

- ERC-AdG, 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).

- ERC-CoG, Controlling Reactive Intermediates in Biocatalysis through Computational Design Tools (BioReInt), - ERC-2025-COG-101232334 was granted to Marc Garcia-Borràs (2026-2031).

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

- COST Action CA21162 (EU-H2020): "COZYME" (2022-2026); M. Garcia-Borràs and S. Osuna were participants.

- COST Action CA21101 (EU-H2020): "COSY" (2022-2026); X. Ribas was participant.

- COST Action CA21126 (EU-H2020): "COSY" (2022-2026); X. Ribas was participant.

- Doctoral Network (EU-H2020): "COMENZE" (2025-2029); S. Osuna was one of the research leaders.

- Doctoral Network (EU-H2020): "HaloVerse" (2026-2030); S. Osuna was one of the research leaders.

- Doctoral Network (EU-H2020): "ELEGANCE" (2026-2029); S. Osuna was one of the research leaders.

- Doctoral Network (EU-H2020): "RADICALLY" (2027-2031); S. Osuna was one of the research leaders.

- FetOpen Consortium (EU-H2020): "FRINGE" (2019-2024); 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 (2020-2024), 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 2022-2025 period are the Dalton Horizon Prize-RSC (2025-Swart), BIOTRANS Junior Award (2025-Osuna) Cadence/OpenEye Outstanding Junior Faculty Award (2024-Garcia-Borràs), Ciamician-González Lectureship Award RSEQ and Italian Chem.Soc. (2023-Costas), EuChemS Lecture Award (2021-Osuna), Bioorg. Chem. Award RSC (2021-Garcia-Borràs). The career trajectories of guarantors and researchers of IQCC were honoured as Fellow of the RSC (2024-Blancafórt, 2024-Solà, 2023-Costas, 2023-Mestres, 2015-Swart), and ChemBioFrance SAB (2023-Mestres).

4) Members of the institute are Keynote/Plenary speakers at prestigious conferences accessible by invitation >160 conferences and at >75 research institutes. S. Osuna (2022 EuChemS conference., and 2022 Solvay conference., 2022 and 2024 Gordon Research Conference), M. Costas (Burgstock conference, 2019), M. Solà (2019 Solvay conference, 2022 Gordon Conference).

5) Leading granted outreach projects at the European level; HORIZON-MSCA-2022-101061189 and HORIZON-MSCA-2024-101162003.

6) Very active international research collaborations (70% of IQCC papers are joint publications with foreign groups).

7) More than 60% of the current IQCC members are from abroad or did the PhD in a foreign Institution (Europe (10 different countries), Asia (3 countries) and America (3 countries)).

8) Members of the unit have participated in 2021-25 in >45 evaluation panels (ERC, FET-OPEN, EIC-Pathfinder, MSCA-PF, MSCA-COFOUND, etc.) and evaluation of ERC proposals (Costas, Swart, Ribas, Poater, Solà, Osuna). IQCC members have acted >270 times as external experts for research proposals, were in >90 PhD reading committees and >10 PhD tribunals, and have reviewed >1565 manuscripts for international scientific journals and as editors of journals (Swart: InorgChimActa; Blancafort: Luminescence, CommunComputSci); Poater: Metal-CentChem, FrontChemTheorComputChem, FrontChemOrganometChem, Science PG; AdvComputChem; IntJMolSci., Catalysts, FrontChem, IndChemMater, IntChinOrgLett; Mestres: ACS MedChemLett; Solà: ACS Omega, ChemSci, AnQuím, TheorChemAcc; Osuna ACS Catal).

9) Member of SAB (Mestres: ChemBioFrance, CAS Life Sci.; Osuna: InstMatAv-UJI; Ribas ISQCH).

Objectives internationalization

For the next five-year period, the objectives for internationalization 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.
- Attract international talent.

Internationalization Actions

1. Increase the participation in international networks. IQCC/IQCS-CAT 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/IQCS-CAT 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/IQCS-CAT through an ICREA contract.
3. Foster the members of IQCC/IQCS-CAT's relations with the international scientific community (organization of conferences, attendance at conferences, ...).
4. Promote the visits of IQCC/IQCS-CAT PhD candidates to foreign labs and the visits of foreign researchers to the IQCC/IQCS-CAT.
5. Increase the number of members of the IQCC/IQCS-CAT with ERC and MSCA grants.
6. Establish a European collaboration network of different groups interested in circular chemistry and sustainability.

Human Capital

The IQCC/IQCS-CAT 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.

General talent attraction and retention

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

General objectives for talent attraction and retention

For the next five-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/IQCS-CAT research groups.

General Actions for talent attraction and retention

1. Pursue the María de Maeztu seal of excellence to attract new PhD candidates and postdocs and to facilitate the retention of researcher manager and technicians.
2. Participate as much as possible in all initiatives related to talent (excellence) recruitment, like those organized by CaixaBank or similar initiatives.
3. Taking external constraints into account, pursue a harmonious growth of the experimental and theoretical parts and the three groups that make up the IQCC/IQCS-CAT.

BSc/MSc students

The IQCC/IQCS-CAT 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 five-year period, the objectives for BSc/MSc students are the following:

- Consolidate the annual Science Slam for attracting new BSc students to the IQCC/IQCS-CAT 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.
3. Promote among IQCC/IQCS-CAT PIs the supervision of Bachelor and Master theses.

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/IQCS-CAT have contributed greatly.

Objectives PhD students

- Consolidate the number of PhD students, and maintain the high level of scientific research that is shown 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 an annual recruitment event at the IQCC/IQCS-CAT level for PhD fellowships provided through research projects.
4. In the context of our transformation to IQCS-CAT, set up annual pre-screening events at the IQCC/IQCS-CAT level for prospective PhD students to apply for competitive fellowships.
5. Allow PhDs to attend at least one international conference per year.

Postdocs

The normal way of entering the IQCC/IQCS-CAT 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 to lead an independent research line and attract funding could be promoted to PI. A recent program of postdoc's mentoring has been started at the IQCC/IQCS-CAT at the beginning of 2026.

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/IQCS-CAT postdocs within the IQCC/IQCS-CAT and outside.

Postdocs Actions

1. Set up annual recruitment event at the IQCC/IQCS-CAT level for postdoc fellowships provided through research projects.
2. Set up annual pre-screening events at the IQCC/IQCS-CAT level for prospective postdocs to apply for competitive fellowships.
3. Promote the research independence of postdocs as a way to facilitate their academic career.

4. Consolidate the ongoing Career Development Plan for non-permanent researchers (Postdocs, Emerging Leaders). Including expectations and fulfillment statements and list of commitments.
5. Establish a Career Evaluation Committee that will periodically (annually) evaluate the performance of non-permanent researchers.
6. Create an Emerging Leader position within the IQCC/IQCS-CAT awarded by the Career Evaluation Committee. An Emerging leader will be the prior step before being promoted to Principal Investigator.
7. Organize annual polls where the researchers can provide opinions on whether the IQCC/IQCS-CAT has satisfied its commitments.

Support staff

The IQCC/IQCS-CAT 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. In case the transformation to IQCS-CAT is carried out, these positions will be covered by the new research center. Similarly, the number of people working as administrative staff will increase and will be covered by the IQCS-CAT.

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 the UdG Rectorate to convince 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 most usual way of entering as a permanent researcher at the IQCC/IQCS-CAT is through a Ramón y Cajal (RyC) contract or with an ICREA senior contract.

Objectives staff

- Incorporate new permanent researchers in the IQCC/IQCS-CAT, with emphasis on experimental sciences to balance the experimental/computational staff ratio, and preferably with an international background.
- Provide necessary means to perform research to all permanent researchers in the IQCC/IQCS-CAT as a way to retain talent.
- Provide permanent positions for Starting Grant and Consolidator Grant researchers and Ramón y Cajal researchers with R3/I3 accreditation.

Staff Actions

1. Modify the policy for attracting Ramón y Cajal 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 R3/I3 accreditation, with permanent positions within the IQCC/IQCS-CAT and Department of Chemistry.
3. Convince the UdG Rectorate of the need to hire RyC researchers who want to join the IQCC/IQCS-CAT.
4. Provide maximum assistance so that IQCC/IQCS-CAT-trained doctors who want to reintegrate into the institute after doing a postdoc 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/IQCS-CAT 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.

6. Make the IQCC/IQCS-CAT an attractive research institute to attract RyCs and ICREA senior researchers.

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 IQCC/IQCS-CAT are also women (42 men and 39 women), although the period 2022-2025, only 12 of the 39 PhD theses that were defended were presented by women. At the staff level, there is still room for improvement. Currently the PIs of the institute consists of 13 men and 3 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.

To monitor and to promote the gender equality, the IQCC/IQCS-CAT has its own gender and diversity committee, which is made up of three PI's and two PhD candidates (*vide infra*).

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 postdoctoral 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/IQCS-CAT 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 postdoctoral 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/IQCS-CAT seminars and at congresses organized by the institute.
- To promote an equal female-male balance of the members serving on evaluation committees (PhD defenses, scientific positions, etc.).

Governance

In the first part of this section, we will show the current governance structure of the IQCC. In the second part, we will discuss the future governance structure of the IQCS-CAT center in case this center is approved. The objectives and actions will be different depending on the new CERCA is approved or not.

The Institute of Computational Chemistry and Catalysis

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 its 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's degree, equivalent to a maximum of 10% of the members of the Institute

Council, and its 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 2026 there are 16 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 they 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 principal investigators committee (DC_{CR}) is made up of the PIs (as of September 2026 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 scientific communication 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, Easter and Summer.
- 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).

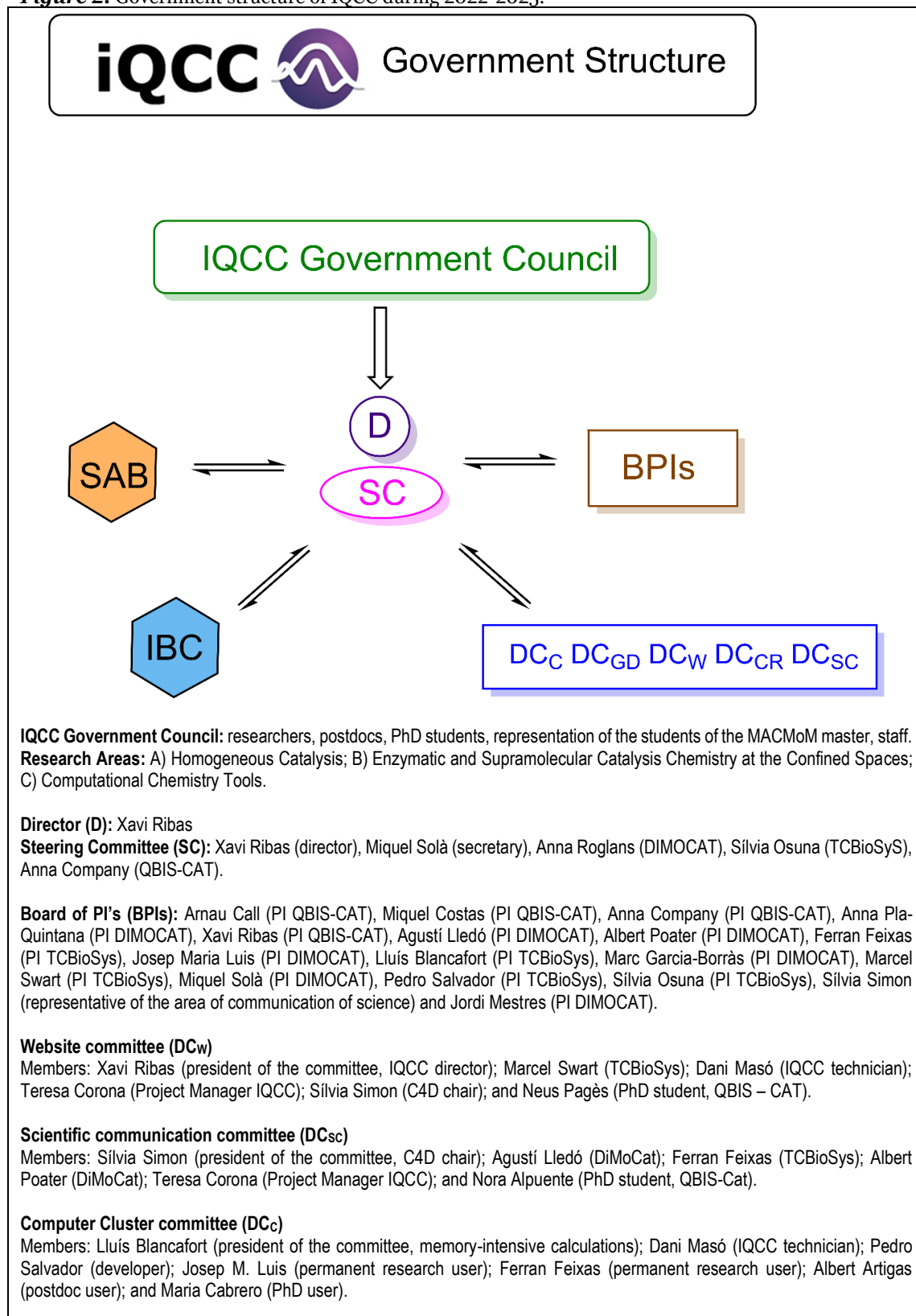
The Scientific Advisory Board (SAB) is the body responsible for advising the scientific policy of the IQCC and for evaluating its activities. The SAB meets every 2 years to evaluate the progress of the IQCC and make scientific suggestions. It was implemented in 2014 and has visited the IQCC six times: in 2014, 2017, 2019, 2021, 2023, and 2025. After the renovation of the members in January 2026, it is composed of nine members selected among prestigious and accomplished professionals in the field of computational chemistry and catalysis. The board is gender-balanced and has five Spanish members and four three 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 four people working in companies with a recognized prestige in the Institute's research fields.

A scheme of the government structure of the IQCC together with the members that form each committee is given in Figure 2.

Figure 2. Government structure of IQCC during 2022-2025.



Computational research committee (DC_{CR})

Members: Agustí Lledó (DiMoCat); Albert Poater (DiMoCat); Ferran Feixas (TCBioSys); Josep Maria Luis (DiMoCat); Lluís Blancafort (TCBioSys); Marc Garcia-Borràs (DiMoCat); Marcel Swart, Miquel Solà (DiMoCat); Pedro Salvador (TCBioSys); Silvia Osuna (TCBioSys).

Gender and diversity committee (DC_{GD})

Members: Anna Company (President, QBIS-CAT); Anna Pla (DiMoCat); Silvia Osuna (TCBioSys); Janet Sánchez (PhD student, TCBioSys, Area B); and Tània Pèlachs (PhD student, QBIS-CAT).

International Business Council (IBC) is the body responsible for advising the technological transfer policy of the IQCC and for evaluating its activities. The IBC meets every 2 years to evaluate the progress of the IQCC and make suggestions. It is currently (June 2026) comprised of the following members: Prof. Xavi Ribas (president of the committee, IQCC director); Dr. Teresa Corona (Project Manager IQCC); Dr. Pere Condom i Vilà (Catalan Government); Dr. Maricel Torrent Jerez (principal researcher at AbbVie, Chicago, USA); Dr. Ester Masllorens Llinas (Senior Vice President Global R&D of Olon Group); and Mr. Jesús Castañón Fernández (Senior Director of Discovery Chemistry and Technologies at the Lilly company in Alcobendas). The ICB was established in 2024.

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 is currently (June 2026) comprised of the following members, selected from amongst prestigious and accomplished academic professionals in the field of computational chemistry and catalysis and from industry: Franziska Schoenebeck (RWTH Aachen University, Germany); Pedro José Pérez Romero (University of Huelva, Spain); Julia Contreras-García (Laboratoire de Chimie Théorique (LCT) Sorbonne Université, CNRS, France); Daniel Maspoch (ICN2, Spain); Carole Duboc (Université Grenoble Alpes and CNRS, France); Vicent Moliner (University Jaume I – INAM, Spain); Araceli González Campaña (University of Granada, Spain); Fernando Cossio (Universidad del País Vasco, Spain); Dr. Enric Comas (Analytics and Digital Lead at UCB, Germany (industry)). The SAB was established in 2014 and has renovated its composition in January 2026. The SAB last met on February 13, 2025, covering the 2023–2024 period, and produced the attached evaluation report. It will meet again in person in early 2027 to discuss mostly the institute, its organization, and committees, with a focus on half of the Pls of the institute.

Since 2017 the IQCC has organized 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 has 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. Since 2023, the IQCC has published its annual scientific report, which can be accessed at the IQCC website.

Finally, since 28 February 2025, the IQCC has an Ethics and Scientific Integrity Committee that is in charge of the resolution of conflicts/actions due to scientific malpractice and problems of scientific integrity at the IQCC and/or ethical conflicts between people working at the IQCC. This committee is an external and independent committee that helps in defining good research practices and research team management, and investigates misconduct complaints submitted by members of the IQCC. It is composed by Dr. Silvia Llach (Associate Professor at the Institute of Research in Education, who is the director), Ms. Núria Frigola (Head of the OITT, who serves as the secretary), Prof. Jordi Poater (ICREA Professor at the Institute of Theoretical and Computational Chemistry (IQTUB) at the University of Barcelona), and Dr. Ester Blay (Head of Gender and Diversity at the Faculty of Law).

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.
- Increase the influence of IQCC in all decisions taken by the UdG government.

Governance Actions

1. Updating the IQCC website by automatizing all online forms and addition of new ones if needed, for efficient internal IQCC procedures.
2. Consolidation of informing IQCC members about administrative procedures, new science policy guidelines, new requirements of Spanish/Catalan governments or European projects.

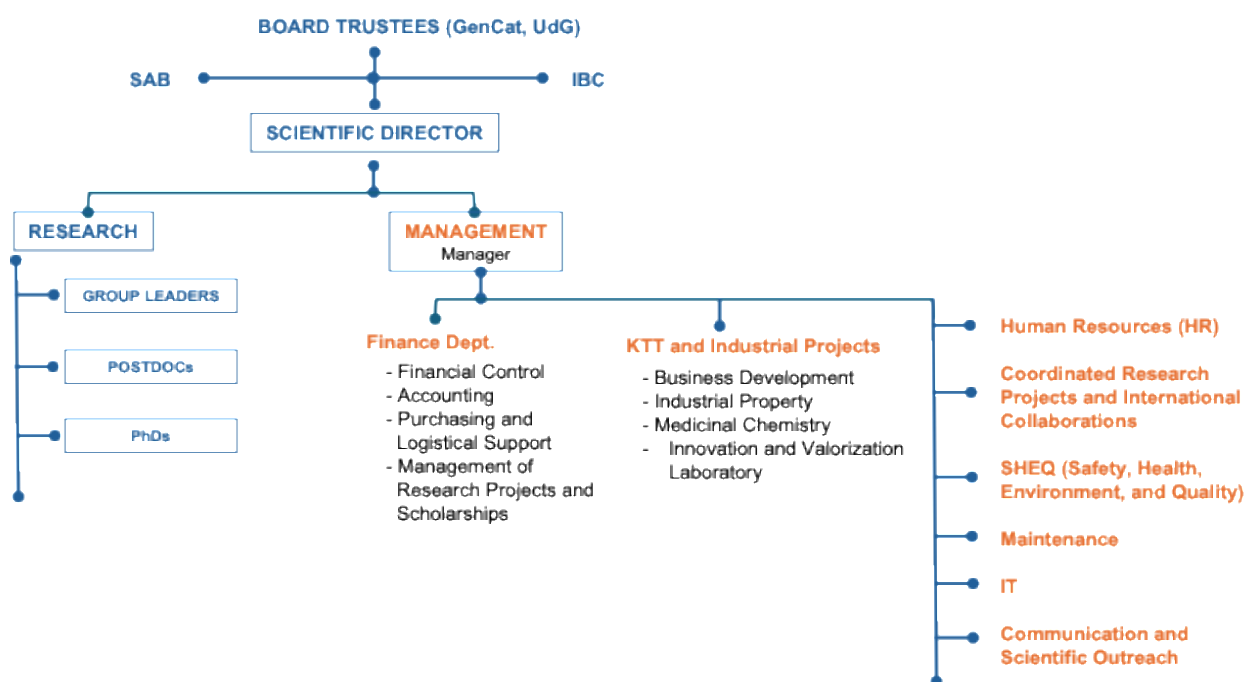
3. Consolidation of efficient decision-making processes within the three-level step process: first discuss in the Steering Committee, then discuss in length in the Board of PIs, and approve formally at the IQCC Council.
4. Study the possibility of incorporating a research group that does not belong to the Department of Chemistry, such as the Protein Engineering Group or the Differential Equations, Modeling and Applications Group to make the IQCC more interdisciplinary.
5. Consider the possibility of creating and launching a delegated experimental research committee (DC_{ER}).
6. Defend before the UdG government that the budget received by the UdG's university institutes and the teaching discounts from the management should be different depending on the size of the institute.
7. As a research center committed to circular chemistry and sustainability, we will create a Sustainability Committee to minimize the environmental impact of our research activities.
8. To have more IQCC members participating in the decision-making body in our university.

The Institute of Circular Chemistry and Sustainability of Catalonia

The government structure of the future Institute of Circular Chemistry and Sustainability of Catalonia (IQCS-CAT) will be the following.

As a legally independent research institute, IQCS-CAT will be governed by its Board of Trustees, to which the SAB, IBC, and the Scientific Director will advise about all relevant matters within the institute. The Scientific Director will be in charge of the research of the institute, including the PI members, junior leaders, postdocs and PhD students. The manager will be responsible for all the financial administration, technical staff members, Human Resources department, and KTT management.

Figure 3. Future government structure of IQCS-CAT.



Objectives Governance

Excellence in research will be pursued. Holding a national or international research grant will be a requisite to be considered a PI of the institute. European projects (individual or via consortium) will be especially welcomed, and the institute will accompany the researchers to submit their applications. Impact and quality in research will be highly valorized over quantity, owing to enhanced international recognition of the institute. Research groups undergoing expansion will be supported by the institute, and additional office and laboratory space will be provided to accommodate their growth. The finance, human resources, and knowledge transfer (KTT) administrative services will be expanded in line with the evolving needs of the institute's research and technical personnel.

Governance Actions

The Institute Manager and the Scientific Director will work in close coordination to ensure the institute maintains a sound and sustainable financial position. They will also engage with the board of trustees to secure fair and appropriate financial support that reflects the institute's size, performance, and scientific excellence.

Infrastructure

The experimental labs have all the necessary equipment for organic and inorganic synthesis and experimental characterization. This includes 5 gloveboxes, 15 chromatographs (GC, GC-MS, HPLC, SC-HPLC, GPC), 3 UV-vis, a FT-IR, an electrochemical work-station, 2 multireactors, 2 high-pressure reactors, a polarimeter, a fluorimeter, 2 ÄKTA GO, a plate reader, a 3D printer, and 2 ion trap mass spectrometers. 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 °C). 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 600 MHz NMR (to be installed by the end of 2026) spectrometers, one X-ray monocrystal 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 recent years, we have had access to resonance Raman equipment (W. Browne, U. of Groningen); spectrofluorimetry equipment (P. Ballester, ICIQ); isothermal titration calorimetry (ITC, E. Palomares, ICIQ); a single-axis diffractometer (D. MasPOCH, ICN2); EPR equipment (C. Duboc Toia, CEA Grenoble and Alex Guo, Carnegie Mellon U.), IR-MS (J. Roithova, Raboud U.), and Mössbauer spectroscopy equipment (A. Guo, CMU, and S. Ye, MPI Mulheim).

As to the computational facilities, the unit has a CPU cluster (Beta) with 89 nodes with a dual processor and a total of 2188 cores, a GPU cluster (Galatea) of 22 nodes with a total of 176 GPUs and another GPU cluster (Krillin) of 12 nodes containing 96 GPUs. 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 (5,5 M hours in 2025 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 83 projects corresponding to 74.12 M hours (2022-2025 period).

At this moment, we are in the process to build a new data processing center (CPD). We have formulated the needs, we have the budget and we are waiting for the different companies to send their offers. We expect the new CPD to solve all problems that we have with the current CPD (related to the high temperatures in summer).

Objectives Infrastructure

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

Governance Actions

1. Setup of the new data processing center (CPD) of the IQCC/IQCS-CAT.
2. Make a list of research equipment needed by IQCC/IQCS-CAT researchers but not available yet.

3. Apply to all possible infrastructure calls to get financial support for new research equipment.

Building

Regarding the space, the IQCC occupies more than 2000 m² of laboratory and office space distributed in a scattered manner between the Faculty of Sciences (in different buildings and corridors) and the Science and Technology Park (Parc-UdG) (Casademont, Giroemprèn, 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/IQCS-CAT or Chemistry Department building.

Governance Actions

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