



STRATEGIC PLAN

OF THE INSTITUTE OF

COMPUTATIONAL CHEMISTRY

AND CATALYSIS

May 2015

This strategic plan follows the recommendations of the report of the Scientific Advisory Board (SAB) from January 2014. It is envisaged for the next three-year period and is divided in the following 8 areas:

- Strategic Research Program
- Organization
- Talent Promotion, Attraction and Retention
- Management and Economy
- Internationalization
- Master and Doctoral Training
- Science Dissemination and Technology Transfer
- Promotion of Gender Equality

Area 2. Strategic Research Program

Current situation

The current scientific structure of the IQCC **has 8 senior research teams** and four junior research teams focusing on four main topics: the development of bioinspired catalysts to perform faster reactions of industrial interest in an environmentally respectful way; the design of efficient catalysts to capture solar energy; the development of new theoretical methods and tools to predict and interpret molecular structure and properties; and the simulation and rational design of molecules and reactions. This structure originates from the merging of the Institut of Computational Chemistry and the METSO and the QBIS research teams.

The forthcoming Strategic Research Program of the institute will recognize **currently active research lines** and will establish **general lines of interest** to which investigators are encouraged to direct their research efforts in the next three year period. The strategic research program will be proposed by the Steering Committee (see Area 2) of the institute, following the evaluation and suggestions of the SAB, on a three year basis. It is the interest of the institute to promote consolidation of the research lines directed by young members that show elements of excellence, and that could help in increasing the international recognition and scientific capabilities of the institute.

General lines of interest

The three general lines of interest for the 2015-2018 period are the following:

a) **The development of new approaches in computational chemistry necessary to bridge the gap between theory and experiment**
b) Evolution towards more sustainable production methods via establishing **homogeneous catalysis methodologies with novel or alternative selectivities**.
c) To establish **methodologies for conversion of light energy into chemical bonds, providing tools in the field of sustainable energies**.

Active research lines

Active research lines of the institute will include **Consolidated Investigator Research Lines** (CIRL) and **Junior Investigator Research Lines** (JIRL). CIRL will be lead by an investigator with a permanent position, while JIRL will be lead by young investigators not holding permanent positions. Any research line will be lead by an investigator of the IQCC and will be uniquely associated to a funded competitive project from a National or International program. Any funded project will be uniquely associated to a single research line, except in the case where the project includes a co-PI. In such cases the project could be associated to two research lines. The existence of the funded project is a requisite for the recognition of a research line. In the case that a research line loses its funding, a period of two years will open for funding to be recovered. After

this time, if absence of funding persists, the line will not be considered as an active research line. A member of the institute responsible for a new funded research project can request the possibility to immediately open an active research line. The Steering Committee will consider the request and can grant preliminary recognition that will be definitively accepted after consideration by the IQCC Council.

Current Active Research Lines are;

1) Simulation of Excited States and Charge Transfer Processes.
   IP: Lluis Blancafort (CTQ)
2) Transition-metal catalyzed cyclization reactions: methodology and mechanisms
   IP: Anna Roglans (CTQ)
3) Spin state catalysis based on density consistent molecular modeling
   IP: Marcel Swart (CTQ, COST Action CM1305)
4) Computational design of proficient enzymes: exploring the molecular basis of biocatalysis (CTQ and CIG)
   IP: Silvia Osuna
5) Biologically inspired design of transition metal reactivity and catalysis
   IP: Miquel Costas (CTQ, StG and Consolider)
6) Sustainable C-X and C-H functionalization catalyzed by Cu^{III} species.
   IP: Xavi Ribas (StG)
7) Activation of small molecules and inert C-H bonds
   IP: Xavi Ribas, Anna Company (CTQ)
8) N2O activation with first row transition metals
   IP: Anna Company (CIG)
9) Catalysis and Aromaticity
   IP: Miquel Solà (CTQ)
10) Computational approaches to alkene metathesis
    IP: Albert Poater
11) Design of molecular containers as nanosensors and nanoreactors
    IP: Xavi Ribas and Miquel Costas (Explora)

Besides the active research grants, the institute recognizes an active line dedicated to the outreach diffusion of science.

Research lines will submit a yearly report of research performance that will be translated to the Steering Committee for evaluation. The model of this report will be taken from ICREA Academia evaluation forms.

Every 3 years, a similar 3-year report will be submitted by each research line for evaluation by the SAB. At the same time, the SAB will review the three strategic objectives and will make recommendations for establishing the objectives for the next three year period.

Area 2. Organization

Current situation

There are eight research teams with one 'team leader' per team, who form the Permanent Board. The competences of the Permanent Board are determined by the institute rules, but the Institute Council can delegate its competences to the Permanent Board if it is considered convenient by the Council (see Article 31.2: The Institute Council can delegate the exertion of its competences to the Permanent Board. The favorable vote of the absolute majority of Institute Council members will be necessary to approve the delegation of competences.)

Current distribution of competences (from IQCC rules)

Permanent board

a) Prepare a proposal for the distribution of the ordinary budget of the institute.
b) Propose the Institute Council to inform about the adscription or leave of institute members.
c) Approve the management report presented by the director and informed favorably by the Advisory Board.
d) Organize and distribute the tasks corresponding to the institute.
e) Care about all functional or general issues of the institute.

Institute Council

a) Prepare and approve the memoir of teaching and research activities of the university research institute.
b) Establish its research and teaching plans.
c) Inform on the individual research and teaching plans of its members and their corresponding contracts.
d) Determine the needs of positions of academic and administration and services personnel.
e) Inform on the adscription of academic personnel to the university research institute.
f) Plan the use of the economic resources and establish the directives to administrate them.
g) Elaborate and propose modifications to its rules.
h) Organize and distribute the inherent tasks of the university research institute.
i) Participate in the preparation and execution of the strategic plan of its action lines in the frame of its competences.
j) Approve the proposal of designation of vice-director and institute secretary.
k) Any other function relative to the university research institute that the Statutes of the University of Girona may attribute explicitly to the Council.

Proposed new organization structure

Based on the recommendations of the SAB report (January 2014), the proposal is (1) to create a Steering Committee formed by the director, the vice-director and a third member of the institute, chosen by the director; and (2) to create a Board of PIs. The boards will have the following competences:

Competences of the Steering Committee

a) Prepare and execute the strategic planning of the institute action lines.
b) Establish research goals for the researchers and approve the research and teaching activity reports of the university research institute.
c) Plan the use of the economic resources of the institute and establish the directives to administer them.
d) Determine the needs of positions of academic and administration and services personnel.
e) Propose to the Institute Council to inform about the adscription or leave of institute members.
f) Organize and distribute the tasks corresponding to the institute.
g) Present a yearly report.
h) Carry out informative meetings with the Board of PIs with public minutes, with at least trimestral frequency.

Composition and competences of the Board of PIs

a) The Board of PIs is an advisory board composed by one representative of every research line, one representative of the area of communication of science and one representative of the Master's Board.

b) Its competence is to carry out informative meetings with the Steering Committee, with at least trimestral frequency.

Competences of the Institute Council

The Institute Council retains the following competences:

a) Approve the yearly report of the Steering Committee.
b) Elaborate and propose modifications to its rules.
c) Approve the proposal of designation of the Steering Committee and institute secretary.
d) Inform on the adscription of academic personnel to the university research institute.

Area 3. Talent Promotion, Attraction and Retention

SAB Recommendations

- Describe the professional situation of former IQCC PhD and postdocs.
- Create the basis to promote young scientists' careers. Young scientists need to fight for rising funding. Periodically evaluate their achievements.
- Prioritize the support to different candidates in external calls according to scientific quality of candidates and institute research strategy

Ideas and proposals

Permanent positions

The IQCC will not consider seriously any permanent position based in anything different from ICREA level, high-standing Ramon y Cajal program, and similar competitive European postdoc programs. However, accomplishments like Starting Grants, relevant projects, and similar outcomes may lead indeed to consider researchers for quasi-permanent or permanent posts.

Talent retention

For nonpermanent IQCC researchers, at all levels, the IQCC should write down a (sustainable and reasonable) "expectation statement" and a "fulfillment assessment" to promote young scientists' careers.

- *Expectation statement*: what does the IQCC expect from predoc and postdoc researchers who may be in need of references and may be able to be considered for new posts?
- Expectations should be accompanied by *commitments*: the researcher should commit to goals; the IQCC should commit to help the researcher (office space, expenses, computing time, lab equipment, proper tutoring and overseeing, etc.). The researcher should commit to search for funding within reasonable limits. Moreover, landmarks should be placed at evenly spaced periods.
- *Periodic evaluation*: the researcher and the IQCC should periodically review landmarks and goals.
- *Fulfillment assessment*: how has the predoc or postdoc research performed vs expectations?
- *IQCC grade of fulfillment*. The researcher should provide opinion also on whether the IQCC has satisfied its commitment.

Talent promotion

Non-permanent Ph.D. researchers who have fulfilled the expectation statement should be helped as much as possible to get a promotion within the very IQCC if available, or to enter a high-standing international research group.

Talent attraction

The ideas for talent promotion and retention are in themselves a tool for talent attraction. Scientists (like all people) need to know in advance the goals they are supposed to reach, and the evaluation procedures and landmarks.

Young Ph.D.'s

The IQCC will do its best to allow undergraduate students to carry out research with the different lines of research. For that purpose, allocation of funds should be made to help partially the living costs of undergraduate researchers.

The IQCC should participate as much as possible in all initiatives concerning talent (excellence) recruitment, like those organized by Caixa de Catalunya or similar initiatives.

Young or senior postdocs

The IQCC will help young postdocs to obtain financial help, participate in leading projects, and receive recognitions that provide them with the opportunity to work as researchers in the IQCC or in the research sector in the same regional area.

The normal way of entering the IQCC at the postdoc level will be either the Juan de la Cierva or equivalent program, or the Ramón y Cajal or equivalent program. For that purpose, "expectation statements" will be agreed and evaluated. Any classification of recent Ph.D.'s, young postdocs or postdocs having completed the RyC program must take into account (a) the assessment of the expectation, and (b) the strategic opportunity of the research line where he/she will work.

For permanent positions (professors at UdG), an international selection committee will oversee the selection process, even though the interests and strategic opinion of the IQCC will be stated clearly in the selection requirements.

The IQCC should publicize the ICREA call (or similar programs) as far as filling empty or limited research lines is concerned. Indeed, if a very qualified researcher is interested in joining the IQCC, and the tentative line of research is not specified in the strategic plan, the IQCC should ponder the opportunity benefits of considering such an application.

In any case, IQCC's policies and attitudes towards talent attraction must be aligned as much as possible with governing bodies. The University of Girona should state clearly its policy regarding this subject, so the IQCC may state clearly the expectations of young scientists willing to join the Institute.

The IQCC should do its best to sign an agreement with the University and thus a clear, sustainable multiyear plan to attract Ramón y Cajal scientists, and also for other programs requiring co-financing by the University. The main instrument for this agreement should be this very Strategic Plan. Any financial help by the University should be related, understandably, to the quality of the IQCC research.

The IQCC should also actively lobby governing bodies in the Regional, National and

European administrations, by presenting them the Strategic Plan, and obtaining commitments and suggestions that maximize opportunities to attract and retain talent.

Special consideration for current researchers

Current researchers having excelled in their work will be considered for permanent positions despite their line of research being filled up. If possible, a change in line of research or evolution to funding-prone research should be pondered in these cases.

Letters of support for current researchers will be issued if goals be fulfilled. Those goals will be set by the IQCC government. Letters will differ and contain the relative ordering/position of a researcher among all current and past IQCC researchers, along with a report by the Director according to the ideas of this section of the Strategic Plan.

Recognition

If asked the IQCC will provide letters of assessment for all their researchers. Similar to letters of support for job opportunities, letters for prizes and other recognition and honors will be different and state clearly the assessment of the researcher.

Main Proposed Actions

1. Establish Career Development Plans for young researchers (Ph.D. students and post-docs) with specific research objectives, a yearly evaluation of the achievements, and a plan for support of the career development.
2. Support and promote the stabilization of UdG Ramón y Cajal fellows by the Directory Board.
3. Aim for a specific agreement between the IQCC and the UdG direction (contracte programa) that guarantees the stabilization of future young ERC grantholders.
4. Regulate the support of the Institute to applications of young researchers to excellence calls (eg ICREA) and prizes on the basis of the Career Development Plan.

Area 4 - Management and Economy

4.1 Technical, administrative and services personnel

Current situation

- Administrative personnel: Excessive workload due to the insufficient number (2 persons) and the non-permanent nature of one of the posts.
- Project manager: the current needs of the institute are satisfied, but the position is non-permanent (financed with own project funds).
- Research technicians: The needs of the computational section are satisfied with the current informatics technician (financed with own project funds). Some of the experimental groups have a laboratory technician ((financed with own project funds), but this number is insufficient. In both cases the stabilization of the positions is necessary to guarantee a stable support.

Needs/Objectives

- 2 permanent administrative personnel + the necessary administrative support
- 1 project manager
- 1 informatics technician
- 3 laboratory technicians

Actions

5. Request from the UdG rectorate the stabilization of temporary personnel and an increase in the current support .
6. Improve the coordination between project manager and administrative personnel to improve the administration and management.
7. Improve coordination between project manager and informatics technician regarding the maintaining of the institute website.
8. Include funding for research technicians in project applications.

4.2 Economy

The institute budget provided by the UdG (approximately 10.000 € per year) covers only the running expenses of the institute. The SAB report proposes to create a 'solidarity canon' where the projects of the groups contribute to the institute's budget. From the administrative point of view, this is only feasible for the projects overheads which are made available by the UdG to the groups ('retrocànons'). In 2014, the total overheads of the groups amounted to 43 176 €.

The administration and management of the institute budget shall be a competence of the Steering Committee, but one of its priorities must be funding fellowships for master's and undergraduate students.

Proposed actions

9. Establish an internal canon of 15% for all project overheads from the institute.

Area 5 - Internationalization

Current situation

According to the SAB report, one of the strongest points of IQCC is its high degree of internationalization. This is made evident by the following observations:

- Several IQCC members have obtained their bachelor, master or PhD degree abroad.
  - *Current PhD students with bachelor and/or master degree abroad*: Michela Milan, Abril Castro, Ewelina Haraburda, Juan Pablo Martínez
  - *Postdocs with PhD abroad*: Elise Bernoud, Cedric Colomban, Ilaria Gamba, Vlad Martin, Christopher Whiteoak
  - *Senior professors with PhD abroad*: Lluís Blancafort, Marcel Swart, Alexander Voityuk, Sergei Vyboishchikov
  - *Former postdocs with PhD abroad*: Alexandra Carvalho, Mikael Johansson, Quansong Li, Diego M. Andrada, William Tiznado, Rachel Crespo, Rafael Islas
- *Visitors to/from foreign institutions*. Very frequently IQCC members visit other laboratories to perform short research stays. Moreover, the labs and offices of IQCC frequently host the visit of professors, postdocs or PhD students from abroad.
- *PhD theses with international mention & PhD stays abroad*. Most PhD theses defended in the IQCC have international mention. This is thanks to the short research stays abroad (3 to 6 months) that most PhD students perform during their PhD studies and the international character of the PhD defense juries, which include at least one member from abroad.
- The different research lines of IQCC maintain extensive *international collaborations*. These include:

  Utrecht University – The Netherlands (Klwin Gebbink). University of Groningen – The Netherlands (Browne). Leibniz Institute for Catalysis Rostock – Germany (Beller). MPI Mülheim – Germany (Neese, DeBeer). Universität Göttingen - Germany (Meyer). UniCat – Germany (Driess, Ray, Limberg). CNRS – France (Latour, Menage, Duboc, Bourissou, Gomez, Caminade). University of Minnesota – US (Que, Cramer). University Charles III Prague – Czech Republic (Roithóva). Brussels – Belgium (Evano, Geerlings). Mérida - Mexico (Merino). Santiago de Chile - Chile (Toro-Labbé). Ghent – The Netherlands (Bultinck). Amsterdam – The Netherlands (Bickelhaupt, Fonseca Guerra). KAUST - Saudi-Arabia (Cavallo). Trinity College Dublin – Ireland (McDonald). Kalkotta - India (Bas). Uppsala – Sweden (Kamerlin, Ottosson). Belgrade – Serbia (Gruden-Pavlovic). Rochester – US (Bren). Durham – UK (Tozer, Verlet). Temple University – US (Perdew). UCLA – US (Houk). CNRS Montpellier – France (Eisenstein, Gatti). Manchester – UK (de Visser). UTEP College of Science – US (Echegoyen). ETH Zurich – Switzerland (Yoko Yamakoshi). CNR Pisa - Italy (Santoro). CNR Naples - Italy (Improta). University College London - UK (Fielding).
  Scientific Computing & Modelling – SCM, Gaussian Inc., Codexis Inc. (Gjalt Huisman)

Important national collaborations: ICIQ – Tarragona (Kleij, Llobet, Pericàs, Lloret-Fillol), ICN2 – ALBA Synchrotron - Barcelona (Maspoch), Barcelona Supercomputer center, Intelligent Pharma (Ignasi Belda), UAB (Sodupe).

- *International funding*. IQCC receives funding from different agencies including the European Commission, such as: Marie Curie International Outgoing Fellowships – IOF (S. Osuna, I. Garcia-Bosch), Marie Skłodowska-Curie Individual Fellowships (F. Feixas), ERC Starting Grant (M. Costas, X. Ribas), ERC Proof of Concept (M. Costas)
- *International networks*. Several members of IQCC participate in international networds that allow the interaction with research groups from other countries. These include:

  COST actions: IQCC members have participated or participate in the following COST actions: CM1003, CM1204, CM1205, CM1305 (coordinator: M. Swart)

  Groupement de Recherche International between Catalonia & Midi-Pyrénées (GDRI): some IQCC members participate in the international network "Hetero-elements and Coordination Chemistry: from Concepts to Applications (HC3A)" (X. Ribas, M. Costas, A. Pla)
- *International visibility*. IQCC aims at getting international visibility by means of different actions: Càtedra de Cultura Científica i Comunicació digital - C4D, 2.0 technologies (webpage, twitter, blogs), participation in TED talks (TEDxUdG, TEDx Barcelona), biannual organization of the Girona Seminar, participation in international conferences.
- *International awards*. Several IQCC members have received awards at international level, in recognition to their outstanding research. These include: European Young Researcher Award (2014: Z. Codolà, 2010: L. Gómez), Clara Immerwahr Award 2014 (A. Company), MGMS Silver Jubilee Prize 2012 (M. Swart), Dalton Young Researcher Award 2010 (A. Company), Member of Young Academy of Europe (M. Swart).

Objectives

For the next 3-year period, the main objectives of the IQCC are:

- keep the high level of internationalization of the institute
- increase the participation in international networks
- increase international funding
- promote the visit of recognized scientists

Proposed actions

1. **Establish new collaborations**. Potential new international collaborations are: Leibniz Institute for Catalysis Rostock – Germany (Hapke, Drexler), Saudi-Arabia (Basset), Oxford – UK (Governeur), Wuhan – China (Lei), Padova – Italy (Bonchio), MPI Göttingen – Germany (Schwarzer), Leeds - UK (Meech), University of Montana – US (Berryman), Allegheny College Meadville – US (Ams)

2. **Promote research stays of PhD students.** All PhD students at the IQCC should perform 2 to 4-month research stays abroad during their PhD. If research projects cannot cover the expenses of these stays, funding should be sought from national calls (AGAUR, MINECO) or from international networks (STSM in COST actions)
3. **Application for international research funding.** When appropriate, postdocs and senior IQCC members should apply for funding to ERC calls including Starting, Consolidator and Advanced Grants. Other international funding should be considered such as the German Academic Exchange Service –DAAD (A. Roglans).
4. **Increase the participation in international networks.** IQCC should increase its participation in international networks. Apart from the ongoing COST actions, some IQCC members plan to apply for other networks such as: European Training Networks – ETN, Future and Emerging Technologies – FET, Research and Innovation Staff Exchange - RISE.
5. **Girona Seminar.** Following the previous editions, the Girona Seminar should invite international recognized scientists to deliver talks and favour their interaction with IQCC members, including PhD and junior postdocs.
6. **Establish a visitor program (VP)**. Every year a recognized scientist will be invited to Girona to spend one week at the IQCC. He/she will deliver a talk that will be made public to the whole university community and the IQCC researchers will be given the opportunity to exchange ideas with him/her.

Area 6 - Master and doctoral training

Current situation

One of the main objectives of the IQCC is to actively participate in the scientific education and training of our young people, starting at secondary school level but 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 in science.

Up until 2012 the members of the IQCC had been involved in two masters' degrees. The first one, Theoretical and Computational Chemistry, was an inter-university master organised by the UdG, UAB, UB, and URV universities, presenting a theoretical and computational approach to chemistry whereas the second one, Molecular Design & Medicinal Chemistry, which was run exclusively by the UdG, was focused on the training of specialists in the fields of medicinal chemistry and molecular design.

One of the aims of the Strategic Plan of the UdG is to "Incentivate groups with good research potential to actively participate in the offer of masters and doctoral degrees and to implement strategies to attract students and to give the university an international projection." With this in mind the IQCC created a new master's degree in 2013 entitled Master in Advanced Catalysis and Molecular Modelling (MACMoM), which combines the knowledge of the two previously taught degrees. The MACMoM has the aim of providing students with the skills needed to address the design of new synthesis of products based upon processes catalysed by transition metals, integrating the most innovative synthetic routes, and directing students towards a more sustainable, efficient and economical catalytic methodologies. This Master also provides students with the opportunity to develop a more theoretical and computational approach to the subject. It is an internationally oriented course comprising 60 ETCS credits, which is taught entirely in English.

Objectives

- To consolidate the MACMoM master by ensuring that a high number of students are enrolled each year and that the level of teaching is high.
- To achieve recognition for the MACMoM master by the UdG as being of strategic interest for the university itself.
- To identify and contact potential foreign partners to create a high-quality Erasmus Mundus Master program that allows different approaches to catalysis and molecular modelling. This master should enable students and visiting scholars from around the world to engage in postgraduate study at European higher education institutions.
- To work together with public institutions, both of the UdG and the Catalan government, to obtain advice for the creation of the Erasmus Mundus master program.

Strategic actions to promote the MACMoM master's degree:

Design and promote policies to attract and retain young research talent for the master's degree.

Attract students that have studied a Chemistry, Biotechnology, Chemical Engineering and Materials Science degree whether at the UdG or other Spanish or foreign institutions:

1. By publicity campaigns both by the UdG and the IQCC
2. Promoting research grants financed by the IQCC to allow students to undertake the final project of the degree
3. In line with the UdG's promotional policies aimed at increasing the international presence of the university particularly in Latin America, work towards dual-degree programs with Latin American universities and promoting agreements with foreign financing agencies.
4. Promoting student-exchange agreements with European universities
5. Encouraging students who do the master's degree in IQCC research groups to stay to do their doctoral degrees at the IQCC.
6. Attract high-performing students for PhD studies in order to obtain competitive grants.

Incentivise effective knowledge transfer to companies and institutions through the master's degree.

7. To promote agreements with companies working in the chemical sector permitting students to undertake their final projects with them in order to encourage the professional orientation pathway of the degree.
8. After the master's degree, encourage industrially-based doctoral degrees to open up opportunities for IQCC research groups to transfer the knowledge and technologies that they acquire and develop.
9. To facilitate the employability in industry of students who undertake their masters doctorate degrees at the IQCC.

Strategic actions to promote the doctoral training:

1. Establish a training program that prepares PhD students for employment both in academia and the private sector.
2. Involve students in challenging and innovative interdisciplinary research projects.
3. Establish a balanced programme of scientific courses that are complemented by courses and workshops to develop highly specialised skills.
4. Encourage doctoral students to obtain experience in advanced foreign institutions.

5. Encourage the short-term placement of PhD students in industrial and academic settings other than that of the institute itself and host graduate students from other institutions.
6. Encourage PhD students to meet the requirements to be awarded an International Doctorate.
7. Promote both pre-doctoral and post-doctoral research visits to foreign institutions and visits by foreign post-docs to the IQCC.
8. Encourage PhD students to present their results through oral communications and posters at international conferences.
9. Promote the attendance of PhD students at winter and summer schools
10. Require PhD students to actively participate in the interpretation of research results and the drafting of academic papers.
11. Create an individual personal career development plan for each PhD student through the establishment of a Training and Supervision Agreement (TSA) document to be approved by a Training Committee which will monitor annually the progress of each student and make recommendations.
12. Hold regular group meetings in which PhD students are required to introduce both their own research findings and present the state of the art as a result of their screening. All meetings will be in English.
13. Promote agreements with international partners to carry out joint doctorate degrees (at this moment the IQCC has an agreement with the VU Amsterdam and two PhDs are enrolled in a double joint degree).

Other general actions:

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 masters and doctorate programs in accordance with their possibilities.

Area 7 - Science dissemination and technology transfer

Current situation

Science dissemination and communication

The IQCC is an active source of dissemination and communication activities. Two different lines are followed:

- the communication of IQCC itself, by means of corporate research teams of individual researchers;
- and by collaborating with the Chair for Science Culture and Digital Communication (C4D), an offspring of the Institute that deals with innovation in digital science communication and with increasing public awareness of science.

Prof. M. Duran and Dr. S. Simon are very experienced researchers in science outreach and communication. Dr. S. Simon is the director of the Chair for Science Culture and Digital Communication and the PI of all Researchers' Nights organized by the IQCC since 2008.

The Institute has been very active in research and science dissemination during the last years, and has also participated in Science Communication innovation projects. The main research strategic objectives of IQCC are communicated to the public and via Internet by a variety of means and actions, all of them related to the concept of Responsible Research and Innovation.

The following outreach activities are currently being pursued at the institute:

- Science Education: IQCC researchers organize activities to communicate their research to young students, while making STEM disciplines, in particular Chemistry, more attractive. Moreover, they use research outputs to involve schools in a general understanding of physical sciences, not just for the most gifted.
- Public Awareness of Science: The IQCC develops initiatives to increase the positive perception of Science and Chemistry among citizenship. We have a large experience in this field - European Researchers' Night projects coordination and organization are the best known.
- Digital Science Communication and Citizen Science: IQCC connects people using a creative approach, and also communicates the research strategic lines of the IQCC making use of the tools provided by the Internet.
- Building bridges between Research and Higher Education: IQCC promotes Open Online Learning. Online education can be viewed as a special form of Online Communication, so training and teaching at master and doctoral levels go in parallel with dissemination. Furthermore, recent IQCC's research on Science Communication and new ways of online teaching (e.g. Massive Open Online Courses (MOOCs)) allow to take a positive, active stand in the most innovative, digital ways to disseminate, communicate, and deliver education.

Technology transfer

The research developed in the IQCC has led to the following main technology transfer achievements:

- the discovery of active sustainable catalysts with potential broad applicability in various commercial fields
- the development of more accurate computational tools for describing experimental systems of interest.

Objectives

For the next three-year period, the objectives for science dissemination and knowledge 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
- study the feasibility of bringing the developed technologies into pre-commercial stages

Actions

Outreach activities

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 Massive Open Online Courses: Three MOOCs will be delivered in the next three-year period: Science Communication 2.0.1, Magic and Science, and Zero Chemistry (connecting high-school students).
4. IQCC research visibility in internet: IQCC's Internet portal (http://iqcc.udg.edu) will be regularly updated with the new scientific outputs obtained, and will continue to grow and improve its active connection with stakeholders: from businesses and industries to citizens, from schools to other research groups.

Knowledge transfer activities:

5. Market Research: Through a preliminary evaluation, the target market of application of the catalysts belongs to the followings sector: pharmaceutical, chemistry industry, biocatalysis industry, and scientific computing and modeling companies. A deeper study will be done focused in an exhaustive analysis of the potential market niches of the catalysts.
6. Intellectual Property (IP) position and strategy: The present strategic plan takes into account the high potential of the developed catalysts and compounds in different industrial applications, so a specific effort will be devoted in defining an IP Strategy and also in analyzing the best protection models to cover future innovation generated. One person of the Technological Transfer Office of UdG (OITT) will be dedicated in defining the IP Strategy and in the elaboration and management of future patents.
7. Industry/sector contacts: A preliminary study of relevant industrial contacts has already been done by identifying three industrial partners of interest: Potential investors, potential licensees, and technology transfer agents. In the next three-year period specific knowledge transfer agents subcontracted through the Technological Transfer Office of UdG (OITT) will support a first commercial prospecting with industry and investors network.
8. The expected outcomes of this knowledge transfer plan will be the commercial availability of a portfolio of new sustainable catalysts and new computational tools with different applications. On the one hand, these catalysts are expected to raise a broad interest in synthesis both in fine and bulk chemistry; and on the other hand the new computational tools developed should serve to establish new methods and protocols to calculation and modeling, designed to improve existing tools on the market.

Area 8 - Promotion of gender equality

There is growing concern in the EU with regards 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, most PhD students in the Department of Chemistry are also women. In our particular institute, as an example, in the period 2008-2012, 10 of the 17 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 13 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

- To encourage 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 organised by the institute.
- To promote an equal female-male balance of the members serving on evaluation committees (PhD defences, scientific positions, etc.).

In conclusion, the IQCC has adopted the promotion of women in chemistry as a medium-term objective that must be achieved through the promotion of female talent through the removal of obstacles to success rather than through positive discrimination. We can and will strongly support women in the institute staying in science and we actively encourage women to apply for positions that become available in the institution at all levels.