



Annual Scientific Report 2024

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1. Preamble

The second annual report of the Institute of Computational Chemistry and Catalysis (IQCC) of the University of Girona (UdG) containing the most important activities developed by the IQCC during 2024 is presented below. Writing an annual report is a valuable practice that goes beyond fulfilling regulatory requirements. It serves as a tool for communication, reflection, and strategic planning, contributing to the overall success and positive reputation of the institute. The present report is the second one.

As you will see in the next pages, 2024 has been a year plenty of activities in research, education, and science communication. We have successfully defended 10 doctoral theses, which represents ca. 10% of UdG theses. We have once again overcome the barrier of 100 articles, some of which have been published in journals of high scientific reputation: 3 Nat. Chem., 2 Nat. Synth., 2 Nat. Commun., 1 ACS Central Sci., 1 Chem. Soc. Rev., 1 PNAS, 7 JACS, 1 JACS Au, 7 Angew. Chem., 6 Chem. Sci., 4 ACS Catal., etc. We have obtained 19 research awards, incorporated 5 new postdocs and organized two international conferences (15th Girona Seminar and EuroQSAR 2024). We have achieved new research projects, among which the ERC Proof of Concept and the MSCA-Doctoral Network from Prof. Silvia Osuna stands out and equipped a new room for the beta computing cluster. We have approved the 2024–2026 strategic plan. We have published the first annual report of IQCC activity, we have continued with the IQCC networking activity, which helps to establish stronger links between IQCC members, especially among the younger ones, and we have brought back the Christmas lunch. We have had the first meeting of the International Business Council, we have passed the first phase to have become a María de Maeztu unit. We have continued with an intense activity of communication and dissemination of research through C4D. In short, an intense year with plenty of great activities and excellent results.

Finally, I want to congratulate and acknowledge all members of the Institute for their effort and enthusiastic work during 2024.

I hope you enjoy reading this annual report for 2024.

Miquel Solà
Director

2. IQCC members

At the end of the 2024, the institute consisted of 102 researchers (6 full professors, 9 associate professors, 2 ICREA Senior researchers, 3 Ramón y Cajal researchers, 3 ex-professors, 14 postdocs, 65 PhD students) and 7 support staff (1 research manager, 2 technicians, 4 administrative staff). The changes during 2024 have been the following:

New members:

- MSc. Iqra Sarfraz, IF-UdG PhD student (M. Solà group and A. Roglans group)
- Dr. Hugo Marchi, postdoc (A. Lledó group)
- MSc. Piyush Piyush, FPI PhD student (X. Ribas group)
- MSc. Esther Pruna, PhD student (S. Osuna group), start date 15/04/24
- Dr. Arijit Saha, Beatriu de Pinós (A. Poater group), start date 01/05/24
- MSc. Aqza Elza John, FPI PhD student (M. Garcia-Borràs group and F. Feixas group)
- MSc. Gopi Krishnan Ravindran, FPI PhD student (LI. Blancafort group)
- MSc. Hande Abes, FI PhD student (M. Garcia-Borràs group and F. Feixas group)
- MSc. Enrico Chianese, PhD student (M. Costas group)
- MSc. Jordi Busoms, PhD student (J. Mestres group)
- Rosa Trujillo, IQCC secretary
- Dr. Mou Mandal, postdoc (A. Poater group)
- MSc. Arslan Ahmad, PhD student (A. Poater group)
- MSc. Muhammad Ehtisham, FI PhD student (A. Poater group and J. M. Luis group)
- MSc. Rabab Maqsood, FI PhD student (A. Poater group)
- MSc. Omkar Charapale, IF-UdG PhD student (M. Solà group)
- MSc. Joan Grèbol, PhD student (P. Salvador group and E. Matito group)
- MSc. Mario Bonachea, PhD student (S. Osuna group)
- MSc. Eva Prat, PhD student (A. Lledó group and E. Palomares group)
- Núria Castanyer, secretary support, start date 16/09/24
- MSc. Raúl Lago, IF-UdG PhD student (M. Garcia-Borràs group and F. Feixas group)
- MSc. Clara Mauclair, PhD student (A. Poater group and J.L. Renaud group)
- MSc. Mahrou Moshfeghnia, PhD student (A. Poater group)
- MSc. Aythami Soto, PhD student (A. Poater group)
- Dr. Alexander Swoboda, postdoc- Erwin Schrödinger fellowship (S. Osuna group)

Changes:

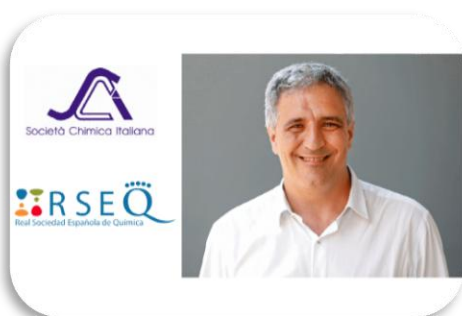
- MSc. Diana Tenica, FI PhD student (M. Costas group)
- Dr. Albert Artigas, postdoc MSCA-PF (M. Solà group)
- Dr. Carles Fuertes, postdoc Beatriu de Pinós (X. Ribas group)
- Dr. Arnau Call, researcher Ramón y Cajal
- Dr. Guillem Casadevall, postdoc (S. Osuna group)

Members that left the Institute:

- MSc. Nicolas Ramírez
- Dr. Ram Mahato, now researcher at Computational and Mathematical Biology Centre (CMBC), India
- Sandra Liu
- Dr. Pau Besalú
- Dr. Elizaveta Petrusevich
- Dr. Sílvia Escayola, now Post-Doc at University of Stuttgart, Germany
- Dr. Christian Curado, now Project Manager UQUIFA, Spain
- Dr. Hugo Valdés, now Assistant professor at Universidad de Alcalá, Spain
- Dr. Stuart Kennington
- Dr. Sarkar Rudraditya, now Assistant Professor at Gandhi Institute of Technology and Management (GITAM), India
- Dr. Antony Stasyuk, now Postdoc at Universitat de Barcelona, Spain
- Dr. Andrea Palone, now Postdoc at Università di Bologna, Italy
- Dr. Àlex Díaz, now Postdoc at Julius-Maximilians-Universität Würzburg, Germany
- Dr. Míriam Pujals
- Dr. Siu-Chung Chan
- Dr. Md Bin Yeamin, now Postdoc at Helmholtz-Zentrum Dresden-Rossendorf (HZDR), Germany
- Dr. Sergio Posada-Pérez, now Postdoc at Catholic University of Louvain, Belgium
- Dr. Yago García-Rodeja
- MSc. Diana Tecnica
- Dr. Jordi Soler, now Postdoctoral at University of Oxford, UK
- Dr. Olga Stasyuk
- Dr. Ouissam El Bakouri, now Postdoc at the Jagiellonian University, Poland
- Dr. Lorena Capdevila

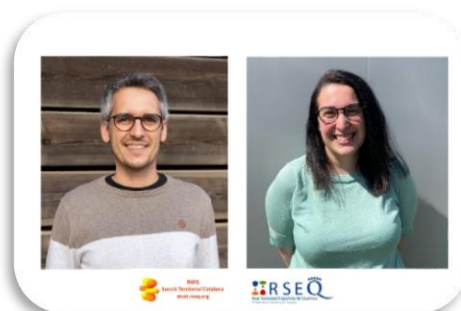
- Dr. Sergi Danés, now Postdoc at the ICIQ, Spain
- Dr. Artur Brotons
- Dr. Marc Montilla

3. Awards and Recognitions



Miquel Costas receives Ciamician-González Lectureship award 2023 - IQCC (udg.edu)

Marc Garcia-Borràs and Laia Vicens receive Marcial Moreno-Mañas Award and Josep Castells award of RSEQ-Cat - IQCC (udg.edu)



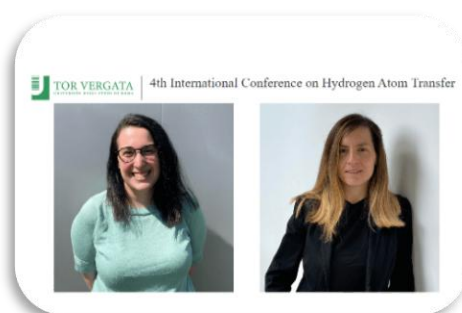
Filippo Scarchilli wins poster prize at the XIV Spanish-Italian Symposium on Organic Synthesis - IQCC (udg.edu)

Sílvia Simon and Miquel Costas receive Communication Award and Scientific Excellence Award 2024 of SCQ - IQCC (udg.edu)



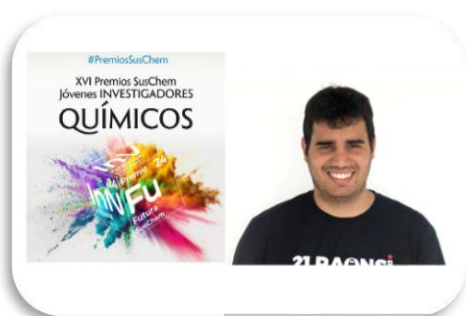
Marc Garcia-Borràs receives Lilly Prize for Young Investigators and Andrea Palone wins RSEQ-Lilly Award for PhD studies - IQCC (udg.edu)

Laia Vicens and Margarida Borrell win poster prize at the 4th International Conference on Hydrogen Atom Transfer - IQCC (udg.edu)



Sílvia Escayola-Gordils selected as one of the six finalists of the European Young Chemists Award 2024 - IQCC (udg.edu)

Martí Gimferrer awarded best PhD thesis 2023 - IQCC (udg.edu)



Jordi Soler receives SusChem Young Chemical Researchers Awards - IQCC (udg.edu)

Mario Bonachea wins poster prize at the IV Jornadas Españolas de Biocatálisis - IQCC (udg.edu)



Ten IQCC researchers have been included in Stanford University global list of 2% top scientists - IQCC

Marc Garcia-Borràs receives the Cadence/OpenEye Outstanding Junior Faculty award - IQCC



Silvia Osuna receives Chemistry Europe Lecture Award (JIQ-RSEQ) - IQCC

Two ICREA Acadèmia awards: Miquel Costas and Miquel Solà - IQCC



Jordi Soler receives PhD theses in Chemistry award of RSEQ-JIQ - IQCC

4. Research visits and invited talks

- Dr. Lluís Artús, Department of Chemistry, KTH Stockholm, 10/01/24
- Prof. Kjell Jorner, Institute for Chemical and Bioengineering, Department of Chemistry and Applied Biosciences, ETH Zürich, 10/01/24
- BSc. Louis A. Van Nyvel, Vrije Universiteit Brussels (M. Solà), 05/02/24-31/07/24

- MSc. Fabio Ioele, Università di Roma Tor Vergata (M. Costas)
- Prof. Alex Zografos, Aristotle University of Thessaloniki (M. Costas), 09/02/24
- Prof. Julia Contreras, Laboratoire de Chimie Théorique, Sorbonne Université/CNRS (P. Salvador), 19/02/24
- Dr. Juan Vicente Alegre-Requena, University of Zaragoza-CISC (M. Garcia-Borràs), 29/02/24
- Dr. Rafael Gramage-Doria, University of Rennes (A. Poater), 29/02/24
- Dr. Carla Casadevall, URV-ICIQ (M. Solà), 07/03/24
- MSc. Eveline Tiekink, Vrije Universiteit Amsterdam (M. Solà), 01/04/24-30/04/24
- BSc. Mehmet Jahja, Université Bourgogne-Franche-Comté (M. Swart), 01/04/24-01/08/24
- BSc. Sami Mahri, Univ. Strasbourg (M. Swart), 15/04/24-28/06/24
- Dr. Maciej Spiegel, Wrocław Medical University (A. Poater), 15/05/24-29/05/24
- Dr. Leo Gross, IBM (M. Solà), 12/06/24
- Prof. Robert S. Paton, Colorado State University (M. Garcia-Borràs, F. Feixas), 13/06/24
- Dr. Heidi Klem, NIST (M. Garcia-Borràs), 21/06/24
- MSc. Alex Iglesias, Nicolaus Copernicus University (J. M. Luis), 15/07/24–18/08/24
- Prof. Yoshiaki Nakao, University of Kyoto, 17/06/24
- MSc. Weronika Bagrowska, Silesian University of Technology- Biotechnology Center (S. Osuna), 19/08/24-31/08/24
- Prof. Tanguy Saget, Institute Chemistry of Substances Natural University Paris-Saclay, 29/08/24
- MSc. Pavel Kohout, Masaryk University (S. Osuna), 01/09/24-30/10/24
- Prof. Aurelio Mateo-Alonso, POLYMAT - University of the Basque Country (M. Solà), 19/09/24
- Dr. Alex Guo, Carnegie Mellon University at Pittsburgh (M. Garcia-Borràs, F. Feixas), 16/10/24
- MSc. Ariadna Pié, DTU (S. Osuna), 26/10/24-20/12/24
- Dr. Alicia Kirk, University of Queensland (M. Garcia-Borràs, F. Feixas), 30/10/24-23/12/24
- Dr. Ping-Yuan Lee, University of Oxford (M. Swart), 04/11/24-09/11/24
- Prof. Michel P. Doyle, University of Texas at San Antonio (A. Roglans, A. Pla-Quintana), 04/11/24
- Prof. Uwe T. Bornscheuer, University of Greifswald (M. Solà), 07/11/24
- MSc. Amira Zgholli, University of Monastir (M. Solà), 07/11/24-07/12/24

- Dr. Massimo Christian D’Alteiro, Università degli Studi di Napoli Federico II (A. Poater), 10/11/24-16/11/24
- Prof. Steven Stevenson, Purdue University Fort Wayne (X. Ribas), 14/11/24
- Prof. Luis Echegoyen, Universitat de Texas – ICIQ (X. Ribas), 15/11/24

5. Research stays

- MSc. David Capellán – CIQSO, Universidad de Huelva (UHU) (Spain), Prof. Pedro J. Pérez, [1 month]
- MSc. Clara Sabrià – Politecnico di Torino (Italy), Prof. Giovanni Pavan, [3 months]
- MSc. Tània Pèlachs – TU Dortmund (Germany), Prof. Guido Clever, [3 months]
- MSc. Faiza Ahsan – Max Plank Institute for Solid State Research (Germany), Dr. Giovanni Li Manni, [3 months]
- MSc. Andrea Álvarez – George-August-Universität Göttingen (Germany), Prof. Franc Meyer, [3 months]
- MSc. Helena Giramé – Technische Universität Berlin (Germany), Dr. Ariane Nunes Alves, [3 months]
- MSc. Abhishek Nair – University College London (UK), Dr. Rachel Crespo-Otero, [3 months]
- MSc. Núria Alsina – Vrije Universiteit Brussel (Belgium), Prof. Mercedes Alonso, [3 months]
- MSc. Janet Sánchez – Silesian University of Technology (Poland), Prof. Artur Góra [2 weeks]
- MSc. Guillem Vila – Donostia Insitute Physics Center (DIPC) (Spain), Dr. Eduard Matito [12 months]
- MSc. Joan Grèbol – Donostia Insitute Physics Center (DIPC) (Spain), Dr. Eduard Matito [24 months]
- MSc. Abhishek Nair – University: University College London (UCL) (UK), Prof. Rachel Crespo-Otero [3 months]
- MSc. Daniel Bosch – King’s College London (UK), Dr. Micaela Matta [3 months]
- MSc. Anju Manickoth – University: Sapienza Università di Roma (Italy), Dr Marco D’Abramo [3 months]
- MSc. Roger Monreal-Corona – Laboratoire de Chimie de Coordination (France), Dr. Rosa Axet, [1 month]

- MSc. Judit Gálvez – Hylleraas Centre for Quantum Molecular Sciences at University of Oslo (Norway), Dr. Marco Bortoli [3 months]
- MSc. Denis Diatlov - Xiamen University (China), Dr. Pavlo O. Dral [4 months]

6. Funding

EU Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
#NitRecerCat2425: La Nit Europea de la Recerca	HORIZON-MSCA-2024-101162003	300.000	S. Simon	01/07/2024 – 30/06/2026
Development of rationally designed enzyme kits	ERC-2023-POC-101158166	150.000	S. Osuna	01/07/2024–31/12/2025
Computational and Experimental Enzyme Engineering for New Polymers	HORIZON-MSCA-2023-DN-101169327	2,563.653 (UdG: 251.971)	S. Osuna	01/03/2025 – 28/02/2029

MICINN Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
Quantum chemistry at the interface between biology, chemistry, materials science and physics	PID2023-152415NB-I00	137.500	M. Swart	01/09/2024 – 31/12/2027
Diseño computacional de compuestos orgánicos pi-conjugados para aplicaciones fotovoltaicas y optoelectrónicas	PID2023-147424NB-I00	237.500	M. Solà	01/09/2024 – 31/12/2028

Espacios confinados quirales para aplicaciones en catálisis asimétrica y materiales quirópticos	PID2023-146498NB-I00	125.000	A. Lledó	01/09/2024 – 31/12/2027
Una aproximación global a la medicina de precisión: de farmacoproteómica a farmacovigilancia	PID2023-153094OB-I00	87.500	J. Mestres	01/09/2024 – 31/12/2027
Desafíos y oportunidades en el control de la selectividad en la ciclación de alenos, fullerenos y vinilcarbenos catalizada por metales	PID2023-146849NB-I00	212.500	A. Pla	01/09/2024 – 31/12/2027
Juan de la Cierva	JDC2023-052336-I	72.000	S. Fernández M. Costas	01/09/2025- 31/08/2027
Juan de la Cierva	JDC2023-052689-I	72.000	E. Masferrer S. Osuna	01/03/2025- 28/02/2027
NMR	EQC2024-008799-P	296.879	STR-UdG	-

AGAUR Funding

Project Title	Reference	Amount (€)	Principal Investigator	Period
Doctorat Industrial	2024 DI 00015	37.800	J. Mestres Chemotargets	01/06/2024- 30/05/2027
Beatriu de Pinós	2022 BP 00051	152.348	A. Saha A. Poater	01/05/2024 – 30/04/2027
Doctorat Industrial	2024 DI 00105	37.800	J. Mestres Chemotargets	2025-2028
Beatriu de Pinós	2023 BP 00033	152.348	A. Artigas M. Solà	2025-2028

ICREA Acadèmia Awards

Project Title	Reference	Amount (€)	Principal Investigator	Period
ICREA Academia 2024	2024 ICREA 00191	200.000	M. Costas	01/01/2025-31/12/2029
ICREA Academia 2024	2024 ICREA 00058	200.000	M. Solà	01/01/2025-31/12/2029

Other Funding

Project Title	Type	Amount (€)	Principal Investigator
EUROPA-UDG2024/15	EUROPA-UdG	3.400	S. Osuna
EUROPA-UDG2024/08	EUROPA-UdG	18.000	M. Solà
EUROPA-UDG2024/10	EUROPA-UdG	15.300	10 Ll. Blancafort
Taula rodona: "Women in Chemical Sciences"	University of Girona – Unitat d'Igualtat	1.000	A. Lledó
5a edició de IQCC open doors 2024	University of Girona – Consell social	1.050	M. Solà
3a edició del Young Researchers Symposium (YRS)	University of Girona – Consell social	1.050	M. Solà
Ciència a la Plaça del Mercat	University of Girona – Consell social	1.050	S. Simon
Campus d'estiu de Màgia i Ciència, 9a edició	University of Girona – Consell social	840	M. Duran
Organització del Congrés Internacional Girona Seminar 2024 (29-31 Maig 2024)	University of Girona – Consell social	1.050	X. Ribas
Intel·ligència Artificial a la Química Computacional: Química Predictiva	University of Girona – Consell social	1.029	A. Poater
PROMOTORS_UdG2023/14	University of Girona	47.850	M. Solà

7. Industrial Collaborations

One of the priorities of the IQCC is to **strengthen the connections with industry**, both nationally and internationally. Apart from projects, collaborations, and research stays of undergrad, Master and PhD students, many of the IQCC Alumni find positions within industry in the participating companies. Furthermore, the IQCC also participates actively in the Industrial Doctorates research *programme* of the *Generalitat de Catalunya*, with several students having already finished their thesis and others have just started on a new joint industry-IQCC PhD thesis.

Fifth IndustryQCC Forum

Last 14th November 2024, the IQCC organized the fifth edition of the IndustryQCC Forum with three national and international companies (**HPCNow, Abbive, and Briolf**) during the Science Week.

The IndustryQCC Forums provide young (and more advanced) researchers of IQCC the opportunity to get to know the research carried out in (bio)chemical industries in different parts of the world; vice versa, for the companies the meetings provide an opportunity to learn about the research of the IQCC, and meet highly qualified researchers with the potential of becoming future employees. This networking activity encourages creating new connections between IQCC/IQCC-researchers and industry in a relaxed and informal manner. This meeting is organized every year since 2020 during the Science Week.

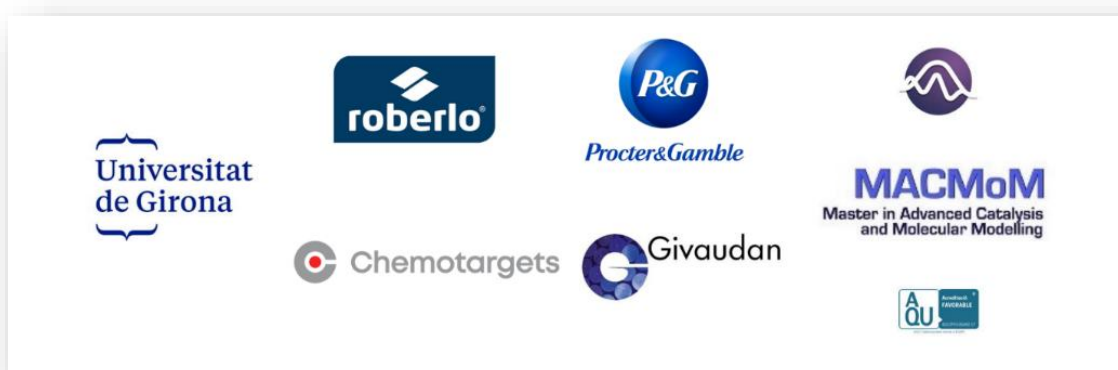
Some companies have shown interest in hosting Master's students for their Master research project and joint research projects have been considered. The event was attended by researchers, postdocs, doctoral students and Master's students from the UdG who were able to speak directly with companies. This facilitated the attraction to the outside world of industry and, at the same time, increases the links between the IQCC and companies to bring research closer to society.







Collaboration with the MACMoM master

During February and March, six of the Master in Advanced Catalysis and Molecular Modelling (MACMoM) students did an internship in [Givaudan](#), [Roberlo](#), [Chemotargets](#) and [P&G company \(Belgium\)](#) to perform their Master research project (TFM) 2023-2024.

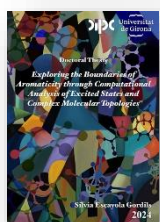
Internship in a company is an optional module of the MACMoM Master, in which the students can perform a full-time internship in a company for up to 4-5 months and a maximum of 750h. In these cases, the Master Thesis is associated with the work carried out in the company, and is co-supervised by a supervisor at the company and a supervisor of the IQCC. The internship corresponds to training undertaken by a student in a national or foreign company, with the aim of applying and complementing the training acquired in the master's degree, bringing the student closer to the reality of the environment in which he/she will exercise his/her professional activity. Every year, some companies have shown interest in hosting Master's students.



New collaboration agreements

Industry	Principal Investigator	Period
Chemotargets  Chemotargets	Albert Poater	2024
SpiroChem AG  SpiroChem <small>GET INSPIRED. INNOVATE.</small>	Miquel Costas	2024
CPTx 	Sílvia Osuna	2024-2024
ArcelorMittal  ArcelorMittal	Miquel Solà	2024-2026

8. PhD tesis



Title: Exploring the Boundaries of Aromaticity through Computational Analysis of Excited States and Complex Molecular Topologies

Author: Escayola Gordils, Sílvia

Directors: Solà, Miquel; Poater, Albert; Matito, Eduard

Defense date: 2024-05-14



Title: Computer-aided design of two-photon-absorbing organic chromophores

Author: Petrusevich, Elizaveta

Director: Luis, Josep M.; Zalesny, Robert

Defense date: 2024-05-14



Title: Oriented external electric fields in chemistry: Development and application of new methods to simulate molecular response properties and reactivity

Author: Besalú Sala, Pau

Director: Luis, Josep M.; Solà, Miquel; Salvador, Pedro

Defense date: 2024-05-20

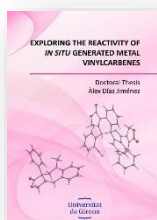


Title: Supramolecular nanocapsules: regioselective functionalization of fullerenes and molecular recognition of endohedral metallofullerenes

Author: Pujals Crusat, Míriam

Director: Ribas, Xavi

Defense date: 2024-06-14



Title: Exploring the reactivity of in situ generated metal vinylcarbenes

Author: Díaz Jiménez, Àlex

Director: Pla-Quintana, Anna; Roglans, Anna

Defense date: 2024-07-15

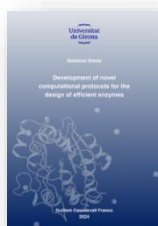


Title: Bio-inspired Manganese-Catalyzed Asymmetric C-H Oxidation: Chiral Pool Expansion and Predictive Data Analysis

Author: Palone, Andrea

Director: Costas, Miquel; Bietti, Massimo

Defense date: 2024-07-30



Title: Development of novel computational protocols for the design of efficient enzymes

Author: Casadevall i Franco, Guillem

Director: Osuna, Sívila; Iglesias-Fernández, Javier

Defense date: 2024-09-13

Title: Main group borohydrides as building blocks - Developing new synthetic methodologies to introduce phosphorus to p- and s- block compounds

Author: Sergi Danés Pibernat

Director: Salvador, Pedro; Andrada, Diego M.

Defense date: 2024-09-30

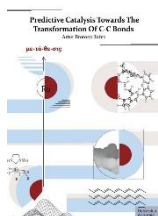


Title: Decomposition of (non)linear optical properties

Author: Montilla Busquets, Marc

Director: Luis, Josep M.; Salvador, Pedro

Defense date: 2024-10-22



Title: Predictive catalysis towards the transformation of C-C bonds

Author: Brotons Rufes, Artur

Director: Poater, Albert; Posada-Pérez, Sergio

Defense date: 2024-11-11

9. Publications

1. S. Sadat Afi Kheljani, K. Didehban, M. Atai, C. Zou, S. Ahmadjo, M. Rodríguez-Pizarro, N. Bahri-Laleh and A. Poater
"In-situ photo-crosslinkable elastomer based on polyalphaolefin/halloysite nanohybrid"
Journal of Colloid and Interface Science **2024**, 659, 751-766
DOI: [10.1016/j.jcis.2023.12.185](https://doi.org/10.1016/j.jcis.2023.12.185)

2. M. Michalak, P. Czerwiński, K. Śniady-Maciażek, S. Musioł, O. Danylyuk, M. Wierzbicki, M. Tomasini and A. Poater
"Chiral NHC Ligands for Enantioselective Gold(I) Catalysis Under Aerobic Conditions: the Importance of Conformational Flexibility and Steric Hindrance of NHC Ligand on Reactivity"
Chemistry A European J. **2024**, *30*, e202303241 DOI: [10.1002/chem.202303241](https://doi.org/10.1002/chem.202303241)
3. P. Hima, M. Tomasini, M. Vagesh, A. Poater and R. Dey
"Access to secondary amines via the hydrogen auto-transfer reaction mediated by K⁺O⁻tBu"
Eur. J. Org. Chem. **2024**, *27*, e202301213 DOI: [10.1002/ejoc.202301213](https://doi.org/10.1002/ejoc.202301213)
4. N. Moeini, H. Teimoury, M. Salimi, N. Bahri-Laleh, M. Joshaghani, J. Duran, A. Poater and S. Posada-Pérez
"Influence of the reaction conditions on the Ziegler-Natta catalyzed ethylene polymerization: Kinetics and properties of the resulting polymers"
Polymer **2024**, *293*, 126640 DOI: [10.1016/j.polymer.2023.126640](https://doi.org/10.1016/j.polymer.2023.126640)
5. M. Orozco-Ic, L. Soriano-Agueda, S. Escayola, D. Sundholm, G. Merino and E. Matito
"Understanding Aromaticity in [5]Helicene-Bridged Cyclophanes: A Comprehensive Study"
J. Org. Chem. **2024**, *89*, 2459-2466 DOI: [10.1021/acs.joc.3c02485](https://doi.org/10.1021/acs.joc.3c02485)
6. R. Carbó-Dorca
"Whole Perfect Vectors and Fermat's Last Theorem"
JAMP **2024**, *12*, 34-42 DOI: [10.4236/jamp.2024.121004](https://doi.org/10.4236/jamp.2024.121004)
7. N. Joly, A. Colella, M. Mendy, M.D. Mbaye, S. Gaillard, A. Poater and J. Renaud
"Blue-Light Induced Iron-Catalyzed Synthesis of γ,δ -Unsaturated Ketones"
ChemSusChem **2024**, *17*, e202301472 DOI: [10.1002/cssc.202301472](https://doi.org/10.1002/cssc.202301472)
8. G. George, A. Poater, M. Solà and S. Posada-Pérez
"Unveiling Oxygen Evolution Reaction on LiCoO₂ Cathode: Insights for the Development of High-Performance Aqueous Lithium-ion Batteries"
Batteries & Supercaps **2023**, *7*, e202300452 DOI: [10.1002/batt.202300452](https://doi.org/10.1002/batt.202300452)
9. S. Escayola, N. Bahri-Laleh and A. Poater
"%V_{Bur} index and steric maps: from predictive catalysis to machine learning"
Chem. Soc. Rev. **2024**, *53*, 853-882 DOI: [10.1039/D3CS00725A](https://doi.org/10.1039/D3CS00725A)
10. A. Shams, F. Karkhaneh, M. Emami, H. Teimoury, H.A. Khonakdar, À. Oliveras, R. Monreal-Corona, A. Pla-Quintana, A. Poater and N. Bahri-Laleh
"Ziegler-Natta catalyst particle size control in propylene/ α -olefin (co)polymerizations"
Molecular Catalysis **2024**, *553*, 113748 DOI: [10.1016/j.mcat.2023.113748](https://doi.org/10.1016/j.mcat.2023.113748)

11. O.A. Stasyuk, M. Solà and A.J. Stasyuk
"Host-guest complexes of perylene bisimide-based metallacage and fullerenes for efficient photoinduced charge separation"
J. Mater. Chem. C **2024**, *12*, 685-695 DOI: [10.1039/d3tc03412g](https://doi.org/10.1039/d3tc03412g)
12. O.A. Stasyuk, A.A. Voityuk, A.J. Stasyuk and M. Solà
"Photoinduced Electron Transfer in Inclusion Complexes of Carbon Nanohoops"
Acc. Chem. Res. **2024**, *57*, 37-46 DOI: [10.1021/acs.accounts.3c00488](https://doi.org/10.1021/acs.accounts.3c00488)
13. N. Choukairi Afailal, M. Borrell, M. Cianfanelli and M. Costas
"Dearomative *syn*-Dihydroxylation of Naphthalenes with a Biomimetic Iron Catalyst"
J. Am. Chem. Soc. **2024**, *146*, 240-249 DOI: [10.1021/jacs.3c08565](https://doi.org/10.1021/jacs.3c08565)
14. A.R. Shaikh, A. Vidal-López, A. Brotons-Rufes, J.J. Pajski, S. Zafar, R.A. Mahmood, M.U. Khan, A. Poater, M. Chawla and L. Cavallo
"Amino acid ionic liquids as efficient catalysts for CO₂ capture: A combined static and dynamic approach"
Results in Surfaces and Interfaces **2024**, *14*, 100175 DOI: [10.1016/j.rsurfi.2023.100175](https://doi.org/10.1016/j.rsurfi.2023.100175)
15. M. Castelli, F. Marchetti, S. Osuna, A.S. F. Oliveira, A.J. Mulholland, S.A. Serapian and G. Colombo
"Decrypting Allosterity in Membrane-Bound K-Ras4B Using Complementary *In Silico* Approaches Based on Unbiased Molecular Dynamics Simulations"
J. Am. Chem. Soc. **2024**, *146*, 901-919 DOI: [10.1021/jacs.3c11396](https://doi.org/10.1021/jacs.3c11396)
16. J.A. Menendez, E. Cuyàs, J.A. Encinar, T. Vander Steen, S. Verdura, À. Llop-Hernández, J. López, E. Serrano-Hervás, S. Osuna, B. Martin-Castillo and R. Lupu
"Fatty acid synthase (FASN) signalome: A molecular guide for precision oncology"
Molecular Oncology **2024**, *18*, 479-516 DOI: [10.1002/1878-0261.13582](https://doi.org/10.1002/1878-0261.13582)
17. C. Castanyer, A. Artigas, N. Insa-Carreras, M. Solà, A. Pla-Quintana and A. Roglans
"Rh-Catalyzed Cycloaddition of C₆₀ with Enynes: Unveiling the Mechanistic Pathway"
Adv. Synth. Catal. **2024**, *366*, 862-869 DOI: [10.1002/adsc.202301189](https://doi.org/10.1002/adsc.202301189)
18. A. Lledó and J. Solà
"The Intermolecular Pauson-Khand Reaction: Applications, Challenges, and Opportunities"
Adv. Synth. Catal. **2023**, *366*, 574-592 DOI: [10.1002/adsc.202301236](https://doi.org/10.1002/adsc.202301236)
19. Y. Rusconi, M.C. D'Alterio, A. Grillo, A. Poater, C. De Rosa and G. Talarico
"The metal role on the activity and stereoselectivity of ring opening polymerization of racemic lactide promoted by Salen catalysts"
Polymer **2024**, *292*, 126639 DOI: [10.1016/j.polymer.2023.126639](https://doi.org/10.1016/j.polymer.2023.126639)

20. B.J. Bloomer, I.A. Joyner, M. Garcia-Borràs, D.B. Hu, M. Garçon, A. Quest, C. Ugarte Montero, I.F. Yu, D.S. Clark and J.F. Hartwig
"Enantio- and Diastereodivergent Cyclopropanation of Allenes by Directed Evolution of an Iridium-Containing Cytochrome"
J. Am. Chem. Soc. **2024**, *146*, 1819-1824 DOI: [10.1021/jacs.3c13011](https://doi.org/10.1021/jacs.3c13011)
21. C. Castanyer, A. Pla-Quintana, A. Roglans, A. Artigas and M. Solà
"Unveiling the regioselectivity of rhodium(I)-catalyzed [2 + 2 + 2] cycloaddition reactions for open-cage C₇₀ production"
Beilstein J. Org. Chem. **2024**, *20*, 272-279 DOI: [10.3762/bjoc.20.28](https://doi.org/10.3762/bjoc.20.28)
22. M. Martinez-Sevillano, M.J. Falaguera and J. Mestres
"CIPSI: An open chemical intellectual property service for medicinal chemists"
Molecular Informatics **2024**, *43*, e202300221 DOI: [10.1002/minf.202300221](https://doi.org/10.1002/minf.202300221)
23. C. Duran, G. Casadevall and S. Osuna
"Harnessing Conformational Dynamics in Enzyme Catalysis to achieve Nature-like catalytic efficiencies: The Shortest Path Map tool for computational enzyme design"
Faraday Discuss. **2024**, *252*, 306-322 DOI: [10.1039/D3FD00156C](https://doi.org/10.1039/D3FD00156C)
24. G. Casadevall, J. Casadevall, C. Duran, S. Osuna and P. Eva
"The shortest path method (SPM) webserver for computational enzyme design"
Protein Engineering, Design and Selection **2024**, *37*, gzae005
 DOI: [10.1093/protein/gzae005](https://doi.org/10.1093/protein/gzae005)
25. J. Ludwig, C. Curado-Carballada, S.C. Hammer, A. Schneider, S. Diether, N. Kress, S. Ruiz-Barragán, S. Osuna and B. Hauer
"Controlling Monoterpene Isomerization by Guiding Challenging Carbocation Rearrangement Reactions in Engineered Squalene-Hopene Cyclases"
Angew. Chem. Int. Ed. **2024**, *63*, e202318913 DOI: [10.1002/anie.202318913](https://doi.org/10.1002/anie.202318913)
26. H. Oh, N. Tumanov, V. Ban, X. Li, B. Richter, M.R. Hudson, C.M. Brown, G.N. Iles, D. Wallacher, S.W. Jorgensen, L. Daemen, R. Balderas-Xicohténcatl, Y. Cheng, A.J. Ramirez-Cuesta, M. Heere, S. Posada-Pérez, G. Hautier, M. Hirscher, T.R. Jensen and Y. Filinchuk
"Small-pore hydridic frameworks store densely packed hydrogen"
Nat. Chem. **2024**, *16*, 809-816 DOI: [10.1038/s41557-024-01443-x](https://doi.org/10.1038/s41557-024-01443-x)
27. V. Iannace, C. Sabrià, Y. Xu, M.v. Delius, I. Imaz, D. Maspoch, F. Feixas and X. Ribas
"Regioswitchable Bingel Bis-Functionalization of Fullerene C₇₀ via Supramolecular Masks"
J. Am. Chem. Soc. **2024**, *146*, 5186-5194 DOI: [10.1021/jacs.3c10808](https://doi.org/10.1021/jacs.3c10808)

28. S. Xu, H. Zhang, J. Xu, W. Suo, C. Lu, D. Tu, X. Guo, J. Poater, M. Solà and H. Yan
"Photoinduced Selective B–H Activation of *nido*-Carboranes"
J. Am. Chem. Soc. **2024**, *146*, 7791-7802 DOI: [10.1021/jacs.4c00550](https://doi.org/10.1021/jacs.4c00550)
29. R. Monreal-Corona, A.J. Stasyuk, M. Solà, A. Pla-Quintana and A. Poater
"Unveiling the reaction mechanisms of the synthesis and the excited state intramolecular proton transfer of 2-(2'-hydroxyphenyl)imidazo[1,2-*a*]pyridine"
ChemPhysChem **2024**, *25*, e202400069 DOI: [10.1002/cphc.202400069](https://doi.org/10.1002/cphc.202400069)
30. C. Maurits de Roo, A.S. Sardjan, R. Postmus, M. Swart, R. Hage and W.R. Browne
"Reaction of (N4Py)Fe with H₂O₂ and the relevance of its Fe(IV)=O species during and after H₂O₂ disproportionation"
ChemCatChem **2024**, *16*, e202301594 DOI: [10.1002/cctc.202301594](https://doi.org/10.1002/cctc.202301594)
31. B. Chandra, F. Ahsan, Y. Sheng, M. Swart and L. Que
"A tale of two topological isomers: Uptuning [Fe^{IV}(O)(Me₄ cyclam)]²⁺ for olefin epoxidation"
Proc. Natl. Acad. Sci. U.S.A. **2024**, *121*, e2319799121 DOI: [10.1073/pnas.2319799121](https://doi.org/10.1073/pnas.2319799121)
32. D.A. Vargas, X. Ren, A. Sengupta, L. Zhu, S. Roy, M. Garcia-Borràs, K.N. Houk and R. Fasan
"Biocatalytic strategy for the construction of sp³-rich polycyclic compounds from directed evolution and computational modelling"
Nat. Chem. **2024**, *16*, 817–826 DOI: [10.1038/s41557-023-01435-3](https://doi.org/10.1038/s41557-023-01435-3)
33. A. Fagnano, F. Fratello, R. Paoloni, C. Sappino, O. Lanzalunga, M. Costas, S. Di Stefano and G. Olivo
"Proximity Effects on the Reactivity of a Nonheme Iron (IV) Oxo Complex in C-H Oxidation"
Angew. Chem. Int. Ed. **2024**, *63*, e202401694 DOI: [10.1002/anie.202401694](https://doi.org/10.1002/anie.202401694)
34. V. Motornov, M. Procházka, N. Alpuente, P. Salvador, P. Slavíček, B. Klepetářová, X. Ribas and P. Beier
"Introducing Weakly Ligated Tris(trifluoromethyl)copper(III)"
ChemistryEurope **2024**, *2*, e202400004 DOI: [10.1002/ceur.202400004](https://doi.org/10.1002/ceur.202400004)
35. M. Saletti, M. Paolino, J. Venditti, C. Bonechi, G. Giuliani, S. Lamponi, G. Tassone, A. Boccia, C. Botta, L. Blancafort, F. Poggialini, C. Vagaggini and A. Cappelli
"A Facile Access to Green Fluorescent Albumin Derivatives"
ChemBioChem **2024**, *25*, e202300862 DOI: [10.1002/cbic.202300862](https://doi.org/10.1002/cbic.202300862)
36. A. Grillo, Y. Rusconi, M.C. D'Alterio, C. De Rosa, G. Talarico and A. Poater
"Ring Opening Polymerization of Six- and Eight-Membered Racemic Cyclic Esters for Biodegradable Materials"
IJMS **2024**, *25*, 1647- DOI: [10.3390/ijms25031647](https://doi.org/10.3390/ijms25031647)

37. Hima P., M. Tomasini, A. Poater and R. Dey
"KOtBu Mediated Alcohol Dehydrogenation Strategy: Synthesis of 2-Aryl Quinazolinones"
ChemistrySelect **2024**, 9, e202400468 DOI: [10.1002/slct.202400468](https://doi.org/10.1002/slct.202400468)
38. M. Galeotti, M. Bietti and M. Costas
"Catalyst and Medium Control over Rebound Pathways in Manganese-Catalyzed Methylenic C–H Bond Oxidation"
J. Am. Chem. Soc. **2024**, 146, 8904-8914 DOI: [10.1021/jacs.3c11555](https://doi.org/10.1021/jacs.3c11555)
39. P. Font, H. Valdés and X. Ribas
"Consolidation of the Oxidant-Free Au(I)/Au(III) Catalysis Enabled by the Hemilabile Ligand Strategy"
Angew. Chem. Int. Ed. **2024**, 63, e202405824 DOI: [10.1002/anie.202405824](https://doi.org/10.1002/anie.202405824)
40. Q. Zhao, Z. Chen, J. Soler, X. Chen, J. Rui, N.T. Ji, Q.E. Yu, Y. Yang, M. Garcia-Borràs and X. Huang
"Engineering non-haem iron enzymes for enantioselective C(sp³)–F bond formation via radical fluorine transfer"
Nat. Synth. **2024**, 3, 958-966 DOI: [10.1038/s44160-024-00507-7](https://doi.org/10.1038/s44160-024-00507-7)
41. K.H. Schülke, J.S. Fröse, A. Klein, M. Garcia-Borràs and S.C. Hammer
"Efficient Transferase Engineering for SAM Analog Synthesis from Iodoalkanes"
ChemBioChem **2024**, 25, e202400079 DOI: [10.1002/cbic.202400079](https://doi.org/10.1002/cbic.202400079)
42. A. Inchausti, R. Mollfulleda, M. Swart, J. Perles, S. Herrero, V.G. Baonza, M. Taravillo and Á. Lobato
"Torsion Effects Beyond the δ Bond and the Role of π Metal-Ligand Interactions"
Advanced Science **2024**, 11, 2401293 DOI: [10.1002/advs.202401293](https://doi.org/10.1002/advs.202401293)
43. J. Soler, S. Gergel, S.C. Hammer and M. Garcia-Borràs
"Molecular Basis for Chemoselectivity Control in Oxidations of Internal Aryl-Alkenes Catalyzed by Laboratory Evolved P450s"
ChemBioChem **2024**, 25, e202400066 DOI: [10.1002/cbic.202400066](https://doi.org/10.1002/cbic.202400066)
44. À. Díaz-Jiménez, R. Monreal-Corona, M. Solà, A. Poater, A. Roglans and A. Pla-Quintana
"Synthesis of 1H-Isoindole-Containing Scaffolds Enabled by a Nitrile Trifunctionalization"
ACS Catal. **2024**, 14, 7381-7388 DOI: [10.1021/acscatal.4c00932](https://doi.org/10.1021/acscatal.4c00932)
45. T. Wu, A. Puri, Y.L. Qiu, D. Ye, R. Sarma, Y. Wang, T. Kowalewski, M.A. Siegler, M. Swart and I. Garcia-Bosch
"Tuning the Thermochemistry and Reactivity of a Series of Cu-Based 4H⁺ /4e⁻ Electron-Coupled-Proton Buffers"
Inorg. Chem. **2024**, 63, 9014-9025 DOI: [10.1021/acs.inorgchem.4c00835](https://doi.org/10.1021/acs.inorgchem.4c00835)

46. M. Jirasek, A. Sharma, J.R. Bame, S.H.M. Mehr, N. Bell, S.M. Marshall, C. Mathis, A. MacLeod, G.J.T. Cooper, M. Swart, R. Mollfullada and L. Cronin
"Investigating and Quantifying Molecular Complexity Using Assembly Theory and Spectroscopy"
ACS Cent. Sci. **2024**, *10*, 1054-1064 DOI: [10.1021/acscentsci.4c00120](https://doi.org/10.1021/acscentsci.4c00120)
47. C. Shu, D.W. Szczepanik, A. Muñoz-Castro, M. Solà and Z. Sun
"[K₂(Bi@Pd₁₂@Bi₂₀)]⁴⁻ : An Endohedral Inorganic Fullerene with Spherical Aromaticity"
J. Am. Chem. Soc. **2024**, *146*, 14166-14173 DOI: [10.1021/jacs.4c03024](https://doi.org/10.1021/jacs.4c03024)
48. À. Díaz-Jiménez, A. Roglans, M. Solà and A. Pla-Quintana
"Mechanistic insights into the rhodium catalysed dehydrogenative cycloaddition of cyano-yne-allene substrates"
Org. Chem. Front. **2024**, *11*, 3655-3662 DOI: [10.1039/D4QO00378K](https://doi.org/10.1039/D4QO00378K)
49. G. George and S. Posada Pérez
"Interaction of C₆₀ with methylammonium lead iodide perovskite surfaces: Unveiling the Role of C₆₀ in Surface Engineering"
Chemistry A European J. **2024**, *30*, e202401283 DOI: [10.1002/chem.202401283](https://doi.org/10.1002/chem.202401283)
50. O.A. Stasyuk, A.A. Voityuk and A.J. Stasyuk
"Facilitating Electron Transfer by Resizing Cyclocarbon Acceptor from C₁₈ to C₁₆"
Chemistry A European J. **2024**, *30*, e202400215 DOI: [10.1002/chem.202400215](https://doi.org/10.1002/chem.202400215)
51. S.K. Thakur, N. Roig, R. Monreal-Corona, J. Langer, M. Alonso and S. Harder
"Similarities and Differences in Benzene Reduction with Ca, Sr, Yb and Sm: Strong Evidence for Tetra-Anionic Benzene"
Angew. Chem. Int. Ed. **2024**, *63*, e202405229 DOI: [10.1002/anie.202405229](https://doi.org/10.1002/anie.202405229)
52. R. Pino-Rios, R. Báez-Grez, D.W. Szczepanik and M. Solà
"Designing potentially singlet fission materials with an anti-Kasha behaviour"
Phys. Chem. Chem. Phys. **2024**, *26*, 15386-15392 DOI: [10.1039/D4CP01284D](https://doi.org/10.1039/D4CP01284D)
53. M. Michalak, P. Czerwiński, K. Śniady-Maciażek, S. Musioł, O. Danylyuk, M. Wierzbicki, M. Tomasini and A. Poater
"Chiral NHC Ligands for Enantioselective Gold(I) Catalysis Under Aerobic Conditions: the Importance of Conformational Flexibility and Steric Hindrance of NHC Ligand on Reactivity"
Chemistry A European J. **2024**, *30*, e202303241 DOI: [10.1002/chem.202303241](https://doi.org/10.1002/chem.202303241)
54. C. Zhu, A. Saquet, V. Maraval, C. Bijani, X. Cui, A. Poater and R. Chauvin
"From Stilbenes to carbo-Stilbenes: an Encouraging Prospect"
Chemistry A European J. **2024**, *30*, e202400451 DOI: [10.1002/chem.202400451](https://doi.org/10.1002/chem.202400451)

55. A. Artigas, Y. Carissan, D. Hagebaum-Reignier, H. Bock, F. Durola and Y. Coquerel
"Aromaticity in Semi-Condensed Figure-Eight Molecules"
Chemistry A European J. **2024**, *30*, e202401016 DOI: [10.1002/chem.202401016](https://doi.org/10.1002/chem.202401016)
56. A.J. Stasyuk, J. Poater and H. Ottosson
"A Voyage into Chemical Bonds and Aromaticity"
Chemistry A European J. **2024**, *30*, e202401206 DOI: [10.1002/chem.202401206](https://doi.org/10.1002/chem.202401206)
57. J. Grèbol-Tomàs, E. Matito and P. Salvador
"Can Aromaticity be Evaluated Using Atomic Partitions based on the Hilbert-space?"
Chemistry A European J. **2024**, *30*, e202401282 DOI: [10.1002/chem.202401282](https://doi.org/10.1002/chem.202401282)
58. S. Chan, A. Palone, M. Bietti and M. Costas
"tert-Butyl as a Functional Group: Non-Directed Catalytic Hydroxylation of Sterically Congested Primary C–H Bonds"
Angew. Chem. Int. Ed. **2024**, *63*, e202402858 DOI: [10.1002/anie.202402858](https://doi.org/10.1002/anie.202402858)
59. D. Diao, A. Baidiuk, L. Chaussy, I. De Assis Modenez, X. Ribas, M. Réglie, V. Martin-Diaconescu, P. Nava, A.J. Simaan, A. Martinez and C. Colombari
"Light-Induced Reactivity Switch at O₂ –Activating Bioinspired Copper(I) Complexes"
JACS Au **2024**, *4*, 1966-1974 DOI: [10.1021/jacsau.4c00184](https://doi.org/10.1021/jacsau.4c00184)
60. P. Salvador, E. Ramos-Cordoba, M. Montilla, L. Pujal and M. Gimferrer
"APOST-3D: Chemical concepts from wavefunction analysis"
J. Chem. Phys. **2024**, *160*, 172502 DOI: [10.1063/5.0206187](https://doi.org/10.1063/5.0206187)
61. M. Tomasini, M. Gimferrer, L. Caporaso and A. Poater
"Rhenium Alkyne Catalysis: Sterics Control the Reactivity"
Inorg. Chem. **2024**, *63*, 5842-5851 DOI: [10.1021/acs.inorgchem.3c04235](https://doi.org/10.1021/acs.inorgchem.3c04235)
62. M. Ahmadi, G. Pareras, M.B. Yeamin, K. Amann-Winkel, A. Rimola, A. Poater and S. Seiffert
"Coordination Geometry and Mineralization in Self-Healing Mussel-Inspired Hydrogels"
Chem. Mater. **2024**, *36*, 3345-3358 DOI: [10.1021/acs.chemmater.4c00037](https://doi.org/10.1021/acs.chemmater.4c00037)
63. S.P. Sitkiewicz, R.R. Ferradás, E. Ramos-Cordoba, R. Zalesny, E. Matito and J.M. Luis
"Spurious Oscillations Caused by Density Functional Approximations: Who is to Blame? Exchange or Correlation?"
J. Chem. Theory Comput. **2024**, *20*, 3144-3153 DOI: [10.1021/acs.jctc.3c01339](https://doi.org/10.1021/acs.jctc.3c01339)
64. F. Peccati, E.L. Noey, K.N. Houk, S. Osuna and G. Jiménez-Osés
"Interplay Between Substrate Polarity and Protein Dynamics in Evolved Kemp Eliminases"
ChemCatChem **2024**, *16*, e202400444 DOI: [10.1002/cctc.202400444](https://doi.org/10.1002/cctc.202400444)

65. E.F. Petrushevich, H. Reis, B. Ośmiałowski, D. Jacquemin, J.M. Luis and R. Zaleśny
"One- and two-photon absorption spectra of organoboron complexes: vibronic and environmental effects"
Phys. Chem. Chem. Phys. **2024**, *26*, 13239-13250 DOI: [10.1039/D4CP01089B](https://doi.org/10.1039/D4CP01089B)
66. S. Escayola, E. Jimenez-Izal, E. Matito, J.M. Ugalde, R. Grande-Aztatzi and J.M. Mercero
"Unveiling the quantum secrets of triel metal triangles: a tale of stability, aromaticity, and relativistic effects"
Phys. Chem. Chem. Phys. **2024**, *26*, 12619-12627 DOI: [10.1039/D4CP00484A](https://doi.org/10.1039/D4CP00484A)
67. X. Liu, P. Cui, Y. García-Rodeja, M. Solà and G. Jin
"Formation and reactivity of a unique M...C-H interaction stabilized by carborane cages"
Chem. Sci. **2024**, *15*, 9274-9280 DOI: [10.1039/D4SC01158A](https://doi.org/10.1039/D4SC01158A)
68. M. Chawla, A. Poater, R. Oliva and L. Cavallo
"Unveiling structural and energetic characterization of the emissive RNA alphabet anchored in the methylthieno[3,4-*d*]pyrimidine heterocycle core"
Phys. Chem. Chem. Phys. **2024**, *26*, 16358-16368 DOI: [10.1039/D3CP06136A](https://doi.org/10.1039/D3CP06136A)
69. N. Proos Vedin, S. Escayola, S. Radenković, M. Solà and H. Ottosson
"The n,π^* States of Heteroaromatics: When are They the Lowest Excited States and in What Way Can They Be Aromatic or Antiaromatic?"
J. Phys. Chem. A **2024**, *128*, 4493-4506 DOI: [10.1021/acs.jpca.4c02580](https://doi.org/10.1021/acs.jpca.4c02580)
70. E. Desmedt, I. Casademont-Reig, R. Monreal-Corona, F. De Vleeschouwer and M. Alonso
"Aromaticity in the Spectroscopic Spotlight of Hexaphyrins"
Chemistry A European J. **2024**, *30*, e202401933 DOI: [10.1002/chem.202401933](https://doi.org/10.1002/chem.202401933)
71. N. Pagès-Vilà, I. Gamba, M. Clémancey, J. Latour, A. Company and M. Costas
"Proton-triggered chemoselective halogenation of aliphatic C-H bonds with nonheme Fe^{IV}-oxo complexes"
Journal of Inorganic Biochemistry **2024**, *259*, 112643
 DOI: [10.1016/j.jinorgbio.2024.112643](https://doi.org/10.1016/j.jinorgbio.2024.112643)
72. J. Xu, L. Bonneviot, Y. Guari, C. Monnereau, K. Zhang, A. Poater, M. Rodríguez-Pizarro and B. Albela
"Matrix Effect on Singlet Oxygen Generation Using Methylene Blue as Photosensitizer"
Inorganics **2024**, *12*, 155 DOI: [10.3390/inorganics12060155](https://doi.org/10.3390/inorganics12060155)

73. J. Trouvé, V. Delahaye, M. Tomasini, P. Rajeshwaran, T. Roisnel, A. Poater and R. Gramage-Doria
"Repurposing a supramolecular iridium catalyst via secondary Zn...O...C weak interactions between the ligand and substrate leads to *ortho*-selective C(sp²)-H borylation of benzamides with unusual kinetics"
Chem. Sci. **2024**, *15*, 11794-11806 DOI: [10.1039/D4SC01515K](https://doi.org/10.1039/D4SC01515K)
74. Q. Zeng, Q. Zhou, C. Calvó-Tusell, S. Dai, X. Zhao, M. Garcia-Borràs and Z. Liu
"Biocatalytic desymmetrization for synthesis of chiral enones using flavoenzymes"
Nat. Synth. **2024**, *3*, 1340–1348 DOI: [10.1038/s44160-024-00596-4](https://doi.org/10.1038/s44160-024-00596-4)
75. A. Mansouri, N.G. Hamedani, C. Zou, S. Mousavi, H.A. Khonakdar, N. Bahri-Laleh, M. Rodríguez-Pizarro, A. Brotons-Rufes, S. Posada-Pérez and A. Poater
"Improving Environmental Stress Cracking Resistance of High-Density Polyethylene Grades by Comonomer Addition and Nanocomposite Approach"
Chemistry A European J **2024**, *30*, e202401926 DOI: [10.1002/chem.202401926](https://doi.org/10.1002/chem.202401926)
76. M. Tomasini, M. Voccia, L. Caporaso, M.L. Szostak and A. Poater
"Tuning the Steric Hindrance of Alkylamines: A Predictive Model of Steric Editing of Planar Amines"
Chem. Sci. **2024**, *15*, 13405-13414 DOI: [10.1039/D4SC03873H](https://doi.org/10.1039/D4SC03873H)
77. G. George, A.J. Stasyuk and M. Solà
"Prediction of the ground state for indenofluorene-type systems with Clar's π -sextet model"
Chem. Sci. **2024**, *15*, 13676-13687 DOI: [10.1039/D4SC03465A](https://doi.org/10.1039/D4SC03465A)
78. A. Juvanteny, C. Souilah, R. Quintero, C. García-Bellido, N. Pagès-Vilà, T. Corona, P. Salvador and A. Company
"Unraveling the Mechanism of Hydrogen Atom Transfer by a Nickel-Hypochlorite Species and the Influence of Electronic Effects"
Inorg. Chem. **2024**, *63*, 14325-14334 DOI: [10.1021/acs.inorgchem.4c00360](https://doi.org/10.1021/acs.inorgchem.4c00360)
79. S. Sadjadi, M. Fahimizadeh, N. Bahri-Laleh, M. Bin Yeamin, P. Yuan and A. Poater
"New halloysite-supported bio-based acidic ionic liquid as an efficient catalyst for conversion of fructose to 5-hydroxymethylfurfural: A combined experimental and computational studies"
Journal of Molecular Liquids **2024**, *410*, 125650 DOI: [10.1016/j.molliq.2024.125650](https://doi.org/10.1016/j.molliq.2024.125650)
80. L. Bettoni, N. Joly, I. Mendas, M.M. Mosconiuri, J. Lohier, S. Gaillard, A. Poater and J. Renaud
"Iron-catalyzed synthesis of substituted 3-arylquinolin-2(1H)-ones via an intramolecular dehydrogenative coupling of amido-alcohols"
Org. Biomol. Chem. **2024**, *22*, 6933-6940 DOI: [10.1039/D4OB00649F](https://doi.org/10.1039/D4OB00649F)

81. D. Unjaroen, D.R. Duijnste, M.D.B. Mancini, J. Chen, R. Hage, M. Swart and W.R. Browne
"Role of non-redox innocent ligand units in the oxidation of alcohols with H₂O₂ catalyzed by μ -oxido-diiron(III) bis-phenolato polypyridyl complexes"
Journal of Inorganic Biochemistry **2024**, *260*, 112698
 DOI: [10.1016/j.jinorgbio.2024.112698](https://doi.org/10.1016/j.jinorgbio.2024.112698)
82. S.F. Vyboishchikov
"Solvation Enthalpies and Free Energies for Organic Solvents through a Dense Neural Network: A Generalized-Born Approach"
Liquids **2024**, *4*, 525-538 DOI: [10.3390/liquids4030030](https://doi.org/10.3390/liquids4030030)
83. L. Capdevila, M.T.G.M. Derks, M. Montilla, J.M. Luis, J. Roithová and X. Ribas
"Direct 2,2,2-Trifluoro and 2,2-Difluoroethoxylation of a Model Macrocyclic Ar-H Substrate via Ni-Catalysis"
ChemistryEurope **2024**, *2*, e202400023 DOI: [10.1002/ceur.202400023](https://doi.org/10.1002/ceur.202400023)
84. A. Ghavampoor, N. Bahri-Laleh, S. Sadjadi, M. Nekoomanesh, A. Vahid, J. Duran, M. Spiegel and A. Poater
"A green approach to synthesize polybutene lubricants from mixed C₄ monomers using supported dendritic ionic liquids"
Journal of Molecular Liquids **2024**, *412*, 125814 DOI: [10.1016/j.molliq.2024.125814](https://doi.org/10.1016/j.molliq.2024.125814)
85. A. Lebcir, A. Boukhari, M. Solà and Y. García-Rodeja
"[4+2]-Cycloaddition Reactions to Corannulene Accelerated by η^6 -Coordination of Ruthenium Complexes"
Eur. J. Org. Chem. **2024**, *27*, e202400697 DOI: [10.1002/ejoc.202400697](https://doi.org/10.1002/ejoc.202400697)
86. M. Swart and M. Reimann
"A benchmark study of dioxygen complexes based on coupled cluster and density functional theory"
SciPost Chem. **2024**, *3*, 001 DOI: [10.21468/SciPostChem.3.1.001](https://doi.org/10.21468/SciPostChem.3.1.001)
87. M. Karimi, S. Sadjadi, H. Arabi, N. Bahri-Laleh and A. Poater
"Design and Synthesis of a Novel Catalytic System Based on Pd Supported on Alumina Extrudates for Hydrotreating of PAO Lubricants"
Appl. Organomet. Chem. **2024**, *38*, e7730 DOI: [10.1002/aoc.7730](https://doi.org/10.1002/aoc.7730)
88. M. Tomasini, T.D. Marforio, M. Calveresi, A. Poater and J. Poater
"Computational Insights into the Regioselectivity of 1,3-Dipolar Cycloadditions inside Carbon Nanotubes"
J. Phys. Chem. C **2024**, *128*, 14961-14971 DOI: [10.1021/acs.jpcc.4c03830](https://doi.org/10.1021/acs.jpcc.4c03830)
89. Z. Sun, J. Zong, H. Ren, C. Lu, D. Tu, J. Poater, M. Solà, Z. Shi and H. Yan
"Couple-close construction of non-classical boron cluster-phosphonium conjugates"
Nat. Commun. **2024**, *15*, 7934 DOI: [10.1038/s41467-024-51506-3](https://doi.org/10.1038/s41467-024-51506-3)

90. A. Álvarez-Núñez, R. Sarkar, V. Dantignana, J. Xiong, Y. Guo, J.M. Luis, M. Costas and A. Company
"Intramolecular C–H Oxidation in Iron(V)-oxo-carboxylato Species Relevant in the γ -Lactonization of Alkyl Carboxylic Acids"
ACS Catal. **2024**, *14*, 14183-14194 DOI: [10.1021/acscatal.4c01258](https://doi.org/10.1021/acscatal.4c01258)
91. M. Ahmadi, A. Poater and S. Seiffert
"Decoding Coordination Geometry Enforcement in Metallo-supramolecular Polymer Networks from Macroscopic Rheological Signatures"
Macromolecules **2024**, *57*, 8803–8812 DOI: [10.1021/acs.macromol.4c01380](https://doi.org/10.1021/acs.macromol.4c01380)
92. S. Escayola, J. Labella, D.W. Szczepanik, A. Poater, T. Torres, M. Solà and E. Matito
"From (Sub)Porphyrins to (Sub)Phthalocyanines: Aromaticity Signatures in the UV–Vis Absorption Spectra"
Inorg. Chem. **2024**, *63*, 18251-18262 DOI: [10.1021/acs.inorgchem.4c03139](https://doi.org/10.1021/acs.inorgchem.4c03139)
93. J. Venditti, M. Saletti, M. Paolino, S. Contena, C. Bonechi, G. Giuliani, G. Giorgi, A.C. Boccia, C. Botta, L. Blancafort and A. Cappelli
"Reactivity of a Morita–Baylis–Hillman Adduct Derivative Bearing a Triphenylamine Moiety with Lysine Models"
Chemistry — An Asian Journal **2024**, *19*, e202400617 DOI: [10.1002/asia.202400617](https://doi.org/10.1002/asia.202400617)
94. A. Palone, M. Bietti and M. Costas
"Enzymatic and Bio-inspired Enantioselective Oxidation of Non-activated C-H Bonds"
Synthesis **2024**, ASAP- DOI: [10.1055/a-2403-0760](https://doi.org/10.1055/a-2403-0760)
95. K. Iudanov, N.B. Nechmad, A. Poater and N.G. Lemcoff
"Selective Cross-Metathesis Versus Ring-Closing Metathesis of Terpenes, Taking the Path Less Travelled"
Angew. Chem. Int. Ed. **2024**, *63*, e202412430 DOI: [10.1002/anie.202412430](https://doi.org/10.1002/anie.202412430)
96. L. Pagès, g. Kurpik, R. Mollfulleda, R.A.A. Abdine, A. Walczak, F. Monnier, M. Swart, A.R. Stefankiewicz and M. Taillefer
"Copper-Catalysed Synthesis of (E)-Allylic Organophosphorus Derivatives: A Low Toxic, Mild, Economical, and Ligand-Free Method"
ChemSusChem **2024**, e202401450 DOI: [10.1002/cssc.202401450](https://doi.org/10.1002/cssc.202401450)
97. M. Ramos, M. Solà and A. Poater
"Hydrophenoxylation of alkynes by gold catalysts: a mini review"
J. Mol. Model. **2024**, *30*, 357 DOI: [10.1007/s00894-024-06152-3](https://doi.org/10.1007/s00894-024-06152-3)
98. S. Goswami, K. Gill, X. Yin, M. Swart and I. Garcia-Bosch
"Cu-Promoted *ipso*-Hydroxylation of sp^2 Bonds with Concomitant Aromatic 1,2-Rearrangement Involving a Cu-oxyl-hydroxo Species"
Inorg. Chem. **2024**, *63*, 20675-20688 DOI: [10.1021/acs.inorgchem.4c03304](https://doi.org/10.1021/acs.inorgchem.4c03304)

99. H. Valdés, N. Alpuente, P. Salvador, A.S.K. Hashmi and X. Ribas
"CCC-NHC Au(III) pincer complexes as a reliable platform for isolating elusive species"
Chem. Sci. **2024**, *15*, 17618-17628 DOI: [10.1039/d4sc02999b](https://doi.org/10.1039/d4sc02999b)
100. Ł. Grzesiński, M. Nadirova, J. Guschlbauer, A. Brotons-Rufes, A. Poater, A. Kajetanowicz and K. Grela
"Preserving precise choreography of bonds in Z-stereoretentive olefin metathesis by using quinoxaline-2,3-dithiolate ligand"
Nat. Commun. **2024**, *15*, 8981 DOI: [10.1038/s41467-024-52876-4](https://doi.org/10.1038/s41467-024-52876-4)
101. C. Duran, T. Kinateder, C. Hiefinger, R. Sterner and S. Osuna
"Altering Active-Site Loop Dynamics Enhances Standalone Activity of the Tryptophan Synthase Alpha Subunit"
ACS Catal. **2024**, *14*, 16986-16995 DOI: [10.1021/acscatal.4c04587](https://doi.org/10.1021/acscatal.4c04587)
102. S.K. Bruffy, A. Meza, J. Soler, T.J. Doyon, S.H. Young, J. Lim, K.G. Huseth, P.H. Willoughby, M. Garcia-Borràs and A.R. Buller
"Biocatalytic asymmetric aldol addition into unactivated ketones"
Nat. Chem. **2024**, *16*, 2076–2083 DOI: [10.1038/s41557-024-01647-1](https://doi.org/10.1038/s41557-024-01647-1)
103. T. Pèlachs, C. Sabrià, V. Iannace, I. Imaz, F. Gándara, D. MasPOCH, F. Feixas and X. Ribas
"Supramolecular Mask Regio-Converter: Orthogonal Diels-Alder C₇₀ Bis-Adducts by Mask-Mediated Regioselective Synthesis"
CCS Chem **2024**, 1-28 DOI: [10.31635/ccschem.024.202405057](https://doi.org/10.31635/ccschem.024.202405057)
104. C. Castanyer, A. Artigas, M. Solà, A. Pla-Quintana and A. Roglans
"On the Functionalization of C₆₀ with Vinylallenes Generated *in situ* by Rhodium Catalysis"
Adv. Synth. Catal. **2024**, ASAP DOI: [10.1002/adsc.202401163](https://doi.org/10.1002/adsc.202401163)
105. M. Freiberger, O.A. Stasyuk, M.E. Pérez-Ojeda, L.A. Echegoyen, M. Solà and T. Drewello
"Stability of [10–12]cycloparaphenylene complexes with pristine fullerenes C_{76,78,84} and endohedral metallofullerenes M₃N@C_{78,80}"
Nanoscale **2024**, *16*, 21068-21076 DOI: [10.1039/d4nr02287d](https://doi.org/10.1039/d4nr02287d)
106. M. Staar, L. Ahlborn, M. Estévez-Gay, K. Pallasch, S. Osuna and A. Schallmey
"A Dynamic Loop in Halohydrin Dehalogenase HheG Regulates Activity and Enantioselectivity in Epoxide Ring Opening"
ACS Catal. **2024**, *14*, 15976-15987 DOI: [10.1021/acscatal.4c04815](https://doi.org/10.1021/acscatal.4c04815)
107. H. Doustmohammadi, J. Sanchez, D. i R. Mahato, S. Osuna
"Evolution Enhances Kemp Eliminase Activity by Optimizing Oxyanion Stabilization and Conformational Flexibility"
Chem. Eur. J. **2024**, e202403747 DOI: [10.1002/chem.202403747](https://doi.org/10.1002/chem.202403747)

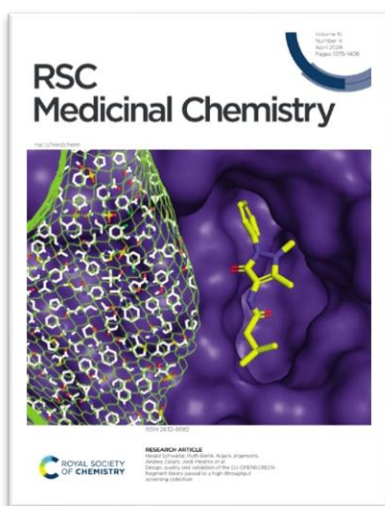
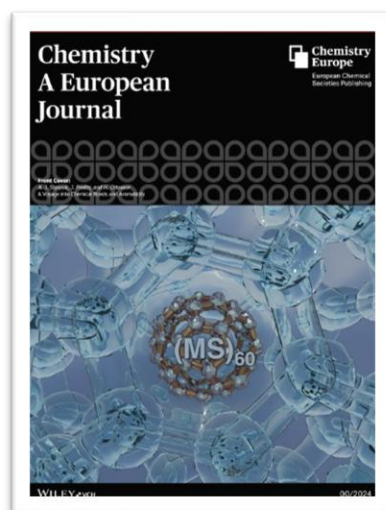
108. J. Wang, Y. Huang, Y. Wang, B. Durbeej, Ll. Blancafort
“Investigating Excited States and Absorption Spectra of the Poly-cyclopentadithiophene-benzothiadiazole Oligomers (Poly-CPDTBT)—A Theoretical Study”
Molecules, **2024**, 29, 5348 DOI: [10.3390/molecules29225348](https://doi.org/10.3390/molecules29225348)
109. D. Ye, T. Wu, A., Puri, D. D. Hebert, M. A. Siegler, M.I P. Hendrich, M. Swart, I. Garcia-Bosch
“Enhanced Proton-Coupled Electron-Transfer Reactivity by a Mononuclear Nickel(II) Hydroxide Radical Complex”
Inorg. Chem., **2024**, 63, 24453–24465

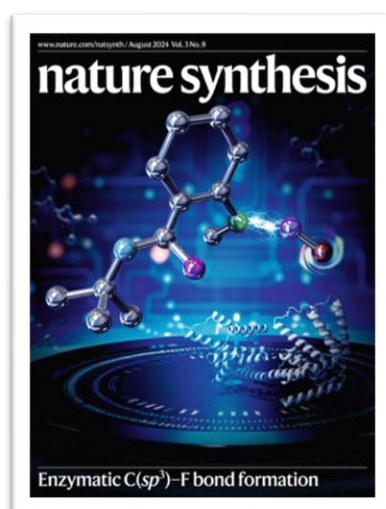
10. Book Chapters

1. Y. García-Rodeja and M. Solà
 “Aromaticity and Antiaromaticity”
 Book: Exploring Chemical Concepts Through Theory and Computation
 DOI: [10.1002/9783527843435.ch9](https://doi.org/10.1002/9783527843435.ch9)
2. A. Artigas, C. Castanyer, A. Roglans, A. Pla-Quintana
 “Functionalization of fullerenes by transition metal catalyzed cyclization reactions: Insights into the mechanisms “
 Book: Advances in Organometallic Chemistry
 DOI: [10.1016/bs.adomc.2024.06.001](https://doi.org/10.1016/bs.adomc.2024.06.001)
3. L. Vicens, M. Costas
 “Activation of hydrogen peroxide with biologically inspired non-heme iron and manganese catalysts: From simple molecular complexes to modification of the second coordination sphere”
 Book: Advances in Inorganic Chemistry
 DOI: [10.1016/bs.adioch.2024.06.001c](https://doi.org/10.1016/bs.adioch.2024.06.001c)
4. R. Carbó-Dorca
 “Conceptual Density Functional Theory-Based Study of Pure and TM s-Doped CdX (X = S , Se , Te ; TMs = Cu , Ag , and Au)”
 Book: Nano Cluster for Water Splitting and Spintronic Applications
 DOI: [10.1002/9781394217656.ch14](https://doi.org/10.1002/9781394217656.ch14)
5. A. Artigas, C. Castanyer, A. Roglans, A. Pla-Quintana
 “Functionalization of fullerenes by transition metal catalyzed cyclization reactions: Insights into the mechanisms”
 Book: Advances in Organometallic Chemistry
 DOI: 10.1016/bs.adomc.2024.06.001

6. C. Duran, G. Casadevall, S. Osuna
 “Harnessing conformational dynamics in enzyme catalysis to achieve nature-like catalytic efficiencies: the shortest path map tool for computational enzyme redesign”
 Book: Faraday Discussions – Biocatalysis
 DOI: 10.1039/D3FD00156C

11. Journal Covers



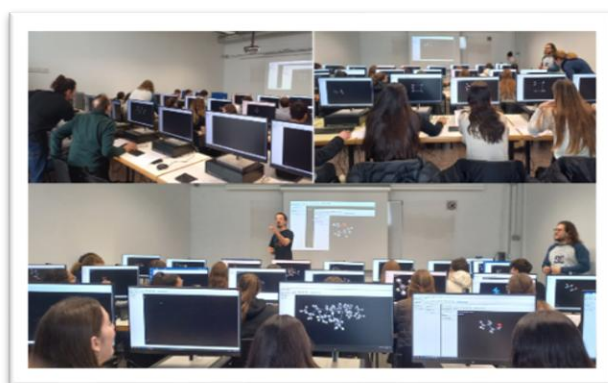


12. Outreach activities

The IQCC is an active source of dissemination and communication activities and has a proven track record in this area. The unit follows two strategies for communication. The first one is direct communication activities of [IQCC](#), by means of corporate platforms (website, social media) and individual promotion by the researchers or research teams. This includes meetings with the general public (e.g. research presentations at high schools). The second one is the alliance with the [Unit for Science Culture and Digital Communication \(C4D\)](#) of the UdG, which is directed by IQCC researcher Dr. Sílvia Simon and can be considered an offspring of the IQCC.

Open IQCC doors to secondary school students 2024

A few times a year, the IQCC opens its doors and gives the opportunity to high-school students to know our work through exciting lectures and computational and experimental workshops. This provides the secondary school pupils the possibility to get a feel for the research and have real-time chemistry in their hands. Last 8th February, it was the turn for the visit of 26 high-school students from INS Narcís Monturiol, 23 of INS Montgrí, 25 INS Celestí Bellera and 21 from INS Josep Brugulat and last 22nd February, it was the turn for the visit of 28 high-school students from INS Montsacopa, 17 of INS Sant Feliu de Guíxols, 35 INS Vallvera and 18 from Montessori Palau Girona.



International Day of Women and Girls in Science at IQCC 2024

11th of February of 2024 was the International day of Women and Girls in Science. The IQCC has currently a rather favourable balance in gender ratio of staff members, both at Master level (54%), PhD level (47%), postdocs (17%) and permanent researchers staff (29%). Notably, out of the 4 most recent permanent members, 2 are men and 2 are women, reinforcing one of the goals of the IQCC of striving to have a gender-balanced permanent staff in the near future.

In order to celebrate this day of the 11th of February, this week Dr. Sílvia Simon presented the STEM film: Madame Curie (Radioactive) (Cinema Trufaut – Girona, 8th Feb). Also, Dr. Sílvia Simon delivered a talk a #100tifiques (Institut Escola Mestre Andreu de Sant Joan les Abadesses) and will participate at TV program La Finestra (Olot TV). Also, Dr. Laia Vicens participated at exposition “Ciència amb Denominació d’Origen Girona; Les nostres veïnes, les nostres científiques” (6-27/02, Girona).

Furthermore, 14 of our IQCC women (Dr. Anna Pla-Quintana, Dr. Sílvia Simon, Dr. Sílvia Osuna, Dr. Anna Roglans, Dr. Olga Stasyuk, MSc. Sílvia Escayola, MSc. Cristina Duran, MSc. Míriam Pujals, MSc. Najoua Choukairi, MSc. Laia Vicens, MSc. Helena Giramé, MSc. Anju Manickoth, MSc. Judit Gálvez, MSc. Núria Alsina) are participating in the International Day of Women and Girls in Science initiative of UdG, where more than 50 researchers are being recognized as #ExpertaUdG.



IQCC Day 2024

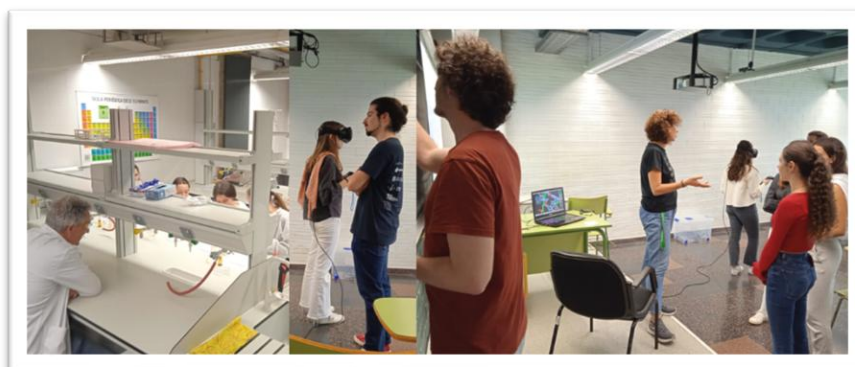
Last Thursday 21st March, the First IQCC Day took place. This activity is part of the Networking IQCC activities. We did an excursion around Estany de Banyoles and then we did a calçotada/BBQ. The idea is that, from now on, we will do once a every year in March.



Chemistry Department open doors 2024

Last 20th March, the Chemistry Department of the University of Girona opened its doors and gives the opportunity to high-school students to know our work through experimental workshops. This provides the secondary school pupils the possibility to get a feel for the research and have real-time chemistry in their hands.

Some IQCC members have participated (Prof. Miquel Costas, Dr. Sílvia Simon, Dr. Ferran Feixas and MSc. Daniel Bosch) with two workshops (virtual reality and IR).



Pint of Science Girona 2024 at IQCC

Every year in May since 2013 the international Print of Science festival is organized. This year was organized by ICREA, IDIBGI, BTM, ERAM, and the Scientific Culture and Digital Communication (C4D) unit of the UdG. Print of Science is an international event with the aim to bring science closer to the general public in a bar. This year, 13-15th of May, the Print of Science took place in Girona. The event will start at 7:30 pm at three different bars (Ateneu Salvadora Catà, Saratoga Cafè and Dolma Lounge). The IQCC will participated with two different talks: on 15th of May at Saratoga Cafè with Prof. Miquel Solà with his talk about “Disseny Molecular per un Futur Energètic Luminós” and with Dr. Marc Garcia-Borràs and his talk about “La química de la biologia a través d’un ordinador”.

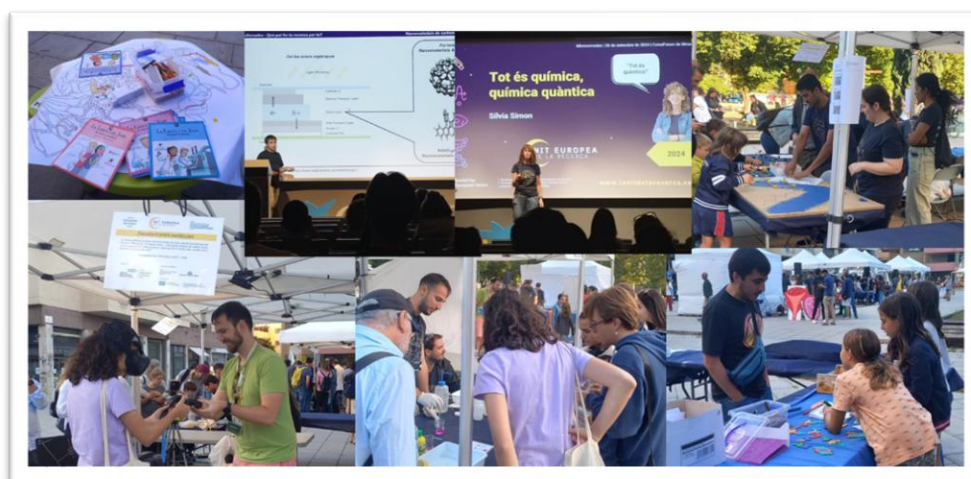


European Researchers’ Night 2024 at IQCC

Every year in September since 2008, the IQCC is organizing together with the Scientific Culture and Digital Communication (C4D) unit of the UdG, the Diputació de Girona and the Girona City Council the European Researchers’ Night with the aim to bring science closer to the Girona general public. The European Researchers’ Night is a coordinated project with Dr. Sívila Simon (researcher of IQCC) and others entities (<https://lanitdelarecerca.cat>).

On September 27, 2024, the European Researchers’ Night took place in Girona. The main event was organized from 5pm to 8pm, where there were different workshops. The IQCC

participated in different ways, **Dr. Sílvia Simon** as organizer, researcher **Prof. Miquel Duran** “Taller d’Intel·ligència Artificial” and “Any Internacional de la Ciència i la Tecnologia Quàntiques” workshops; the postdoctoral and PhD students **Dr. Miquel Estévez-Gay, MSc. Aqza John, MSc. Hande Abes** with the “Passejant entre molècules” and **Dr. Albert Artigas** with “Construeix el teu propi nanografè” workshop; **Dr. Marco Galeotti** and **MSc. Filippo Scarchilli** with the “Catalysis” workshop; **Prof. Lluís Blancafort, Dr. Ouissam El Bakouri, MSc. Judit Gálvez, MSc. Gopi Ravindran, MSc. Anju Manickoth** with the “Porfirines i aromaticitat” workshop; **Prof. Sílvia Osuna, MSc. Jonnelly Luizaga** and **MSc. Cristina Duran** with the “Coloring and drawing” and “What is an enzyme? Stories to save the planet” workshop and **MSc. Daniel Bosch** with “Música i AI”. Furthermore, the researcher **Dr. Sílvia Simon** and the postdoctoral researcher **Dr. Albert Artigas** did a microtalk about “Tot és química, química quàntica!” and “Nano-estructures de carboni per un futur sostenible” at CaixaForum (26th Sept).



IQCC Science Slam 2024

Since 2015 the IQCC is organizing a Science Slam. Last October 1st the IQCC was organized the IX edition to show the most representative research projects of the Institute to a wide audience. The research carried out within each of the research teams of the IQCC was explained briefly summarized by the PIs (2 minutes).



Science Week – Diada de Sant Albert at IQCC and Science Faculty UdG 2024

Every year in November, the IQCC is organizing together with the Scientific Culture and Digital Communication (C4D) unit of the UdG some activities for Science Week with the aim to bring our science closer to the Girona general public.

On November 15, 2024, the Diada de Sant Albert took place at Science Faculty of UdG. The event was organized from 09.00h to 13.00h, where there were different workshops and stands. The IQCC participated in a stand on “Catàlisi: a on la trobem?” by two bachelor students (Fran Puga and Daniel Redondo) to show our chemistry to more than 600 high-school students.



