

## 1. PERSONAL INFORMATION

Family name, First name: Maseras, Feliu

Researcher unique identifiers: B-1002-2008 (Research ID), 0000-0001-8806-2019 (ORCID)

URL for web site: [http://www.iciq.org/research/research\\_group/prof-feliu-maseras/](http://www.iciq.org/research/research_group/prof-feliu-maseras/)

## 2. EDUCATION

1991 PhD in Chemistry. Topic: Computational inorganic chemistry, Universitat Autònoma de Barcelona, Catalonia, Spain

1988 Master in Chemistry  
Universitat Autònoma de Barcelona, Catalonia, Spain

## 3. CURRENT POSITION

2004– Senior researcher, Group leader,  
Institute of Chemical of Research of Catalonia (ICIQ), Tarragona, Catalonia, Spain

## 4. PREVIOUS POSITIONS

1998 – 2019 Associate Professor  
Chemistry Department, Universitat Autònoma de Barcelona, Catalonia, Spain

1996 – 1998 Research Associate  
Laboratoire de Structure et Dynamique de Systèmes Moléculaires et Solides (LSDSMS), Université de Montpellier 2, France

1993 – 1996 Research Associate  
Chemistry Department, Universitat Autònoma de Barcelona, Catalonia, Spain

## 5. FELLOWSHIPS AND AWARDS

2011 Bruker award (Physical Chemistry), received from the Real Sociedad Española de Química

2008 Chemical Society Reviews Lecture award, received from the Royal Chemical Society

2000 Distinction for Young Researchers, received from the Generalitat de Catalunya

1991 – 1993 Institute of Molecular Science, Okazaki, Japan  
Research fellow of the European Communities under the STFPJ Programme

1987 – 1991 Chemistry Department, Universitat Autònoma de Barcelona, Catalonia, Spain  
Research fellow of the Spanish government under the FPI Programme

## 6. SUPERVISION OF GRADUATE STUDENTS AND POSTDOCTORAL FELLOWS

2004 – 2022 15 Postdoctoral Fellows / 18 PhD Students/ 15 Master Students  
Institute of Chemical of Research of Catalonia (ICIQ), Tarragona, Catalonia, Spain

1997 - 2004 6 PhD Students/ 7 Master Students  
Chemistry Department, Universitat Autònoma de Barcelona, Catalonia, Spain

## 7. TEACHING ACTIVITIES

2009 – Professor in Master courses – physical chemistry, Universitat Rovira i Virgili, Tarragona

2008 – 2012 Professor in Master courses – physical chemistry, inter-university training, Catalonia

1998 - 2004 Associate Professor – physical chemistry, undergraduate teaching in Universitat Autònoma de Barcelona

1987 – 1991 Assistant Professor – physical chemistry, undergraduate teaching in Universitat Autònoma de Barcelona

## 8. ORGANISATION OF SCIENTIFIC MEETINGS

- 2018 Chairman, symposium “Computational Catalysis for Sustainable Chemistry”, Spain  
2015 Chairman, “Japan-Spain symposium on theoretical chemistry for complex systems”, Spain  
2015 Chairman, “3rd meeting of the CARISMA COST Action”, Spain  
2013 Chairman, “Dialogue Experience Theory in Inorganic Chemistry 2013”, Spain

## 9. INSTITUTIONAL RESPONSIBILITIES

- 2015 – 2020 Member of Academic Commission, Institute of Chemical of Research of Catalonia  
2008 Responsible for international seminars programme, Institute of Chemical of Research of Catalonia  
2000 – 2004 Member of the direction board in the Department of Chemistry, Universitat Autònoma de Barcelona

## 10. REVIEWING ACTIVITIES

(only those with official appointment letter)

- 2020- Scientific Advisory Board, Hokkaido University, ICRDD, Japan  
2019 – Associate Editor, ACS Catalysis, American Chemical Society  
2011 - Advisory Editorial Board, Chemical Society Reviews, Royal Society of Chemistry  
2012 – 2015 Review panel member, “Agencia Nacional de Evaluación y Prospectiva”, Spain  
2009 – 2010 Review panel member, “Agencia Andaluza de Evaluación”, Andalusia, Spain  
2008 – 2010 Evaluation committees for three institutions, AERES, France

## 11. MEMBERSHIPS OF SCIENTIFIC SOCIETIES AND RESEARCH NETWORKS

- 2015 - Member, Research Network “Hetero-elements and Coordination Chemistry: from Concepts to Applications (HC3A)”  
2014 – 2017 Member, Research Network “Catalytic Routines for Small Molecule Activation” (COST Action)  
2007 – Member, “Real Sociedad Española de Química”  
2000 – Member, American Chemical Society

## 12. HIGHLIGHTS FROM RESEARCH 2015-2024

### Top 5 publications on computational homogeneous catalysis

1. *Redox Non-innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts*  
P. Garrido-Barros, I. Funes-Ardoiz, S. Drouet, J. Benet-Buchholz, F. Maseras, A. Llobet *J. Am. Chem. Soc.*, **137**, 6758-6761 (2015)  
The proposal of a new mechanism for water oxidation, in collaboration with the experimental group of Llobet (ICIQ)
2. *Stereoselective and Versatile Preparation of Tri- and Tetra-Substituted Allylic Amine Scaffolds under Mild Conditions*  
W. S. Guo, L. Martínez-Rodríguez, R. Kuniyil, E. Martín, E. C. Escudero-Adan, F. Maseras, A. W. Kleij *J. Am. Chem. Soc.*, **138**, 11970-11978 (2016)

The clarification of the mechanism for a synthetic process in collaboration with the experimental group of Kleij (ICIQ)

3. *Oxidative coupling mechanisms: Current state of understanding*  
I. Funes-Ardoiz, F. Maseras *ACS Catal.* **8**, 1161-1172 (2018)  
A review on the mechanism for oxidative coupling.
4. *Scope and Challenge of Computational Methods for Studying Mechanism and Reactivity in Homogeneous Catalysis*  
J. N. Harvey, F. Himmo, F. Maseras, L. Perrin *ACS Catal.*, **9**, 6803-6813 (2019)  
A review with four corresponding authors on the right way to do computational homogeneous catalysis.
5. *Charge-Controlled Pd-Catalysis Enables the Meta-C-H activation and olefination of arenes*  
A. Mondal, M. Díaz-Ruiz, F. Deufel, F. Maseras, M. van Gemmeren  
*Chem*, **9**, 1004-1016 (2023)  
The report of a new method for the selective activation of the meta C-H bond of arenes, in collaboration with the experimental group of van Gemmeren (Kiel)

#### **Top 5 publications beyond homogeneous catalysis**

1. *Managing the Computational Chemistry Big Data Problem: The ioChem-BD Platform*  
M. Alvarez-Moreno, C. de Graaf, N. Lopez, F. Maseras, J. M. Poblet, C. Bo *J. Chem. Inf. Model.*, **55**, 95-103 (2015)  
The presentation of the ioChem-BD repository for computational results. A collaboration with four other computational research groups based in Tarragona.
2. *Microkinetic modeling in homogeneous catalysis*  
M. Besora, F. Maseras *WIREs Comp. Mol. Sci.*, **8**, e1372 (2018)  
A review on the application of microkinetic models by us and others.
3. *The challenge of reproducing with calculations raw experimental kinetic data for an organic reaction*  
R. Pérez-Soto, M. Besora, F. Maseras *Org. Lett.*, **22**, 2873-2877 (2020)  
A discussion on the use of tuning for reaching agreement between calculation and experiment
4. *Understanding ball milling mechanochemical processes with DFT calculations and microkinetic modelling*  
B. S. Pladevall, A. de Aguirre, F. Maseras *ChemSusChem*, **14**, 2763-2768 (2021)  
Our initial work on mechanochemistry.
5. *Hidden descriptors: Using statistical treatments to generate better descriptor sets*  
L. Morán-González, F. Maseras *Artificial Intelligence Chemistry.*, **3**, 100061 (2024)  
A review on our hidden descriptor approach for the generation of better descriptor for machine-learning treatments

#### **Publications summary (Web of Science, April 2024)**

106 publications in peer-reviewed scientific journals since January 2015 (12 in *J. Am. Chem. Soc.*, 8 in *Angew. Chem. Int. Ed.*, 13 in *ACS Catal.*, 8 in *Chem. Eur. J.*, 2 in *Chem. Commun.*, 2 in *Chem. Sci.*, 1 in *WIREs Comp. Mol. Sci.*, 1 in *Nature Catal.*, 1 in *Nature Chem.*, 1 in *Chem*, 6 in *Organometallics*, 2 in

*Inorg. Chem.*, 2 in *ChemCatChem*, 3 in *Dalton Trans.*, 3 in *Org. Lett.*, 1 in *Catal. Sci. Technol.*, 2 in *J. Chem. Inf. Mod.*, 1 in *Chem Catalysis*, 1 in *ChemSusChem*, 1 in *JACS Au*). A total of 2,769 citations (h = 28) for papers published since 2015.

Out of a total of 314 publications since 1989, with 15,635 total citations, total h index 62. One publication (*J. Comput. Chem.* 1995) with over 1,500 citations, 10 other publications over 200 citations, a total of 38 publications over 100 citations.

### **Top 5 invited presentations**

1. 253<sup>rd</sup> ACS National Meeting, San Francisco, April 2017
2. 16<sup>th</sup> International Congress of Quantum Chemistry (ICQC-2018), Menton (France), June 2018
3. International Forum on Green Chemistry, Wenzhou (Zhejiang, China), October 2019.
4. 10th International Conference on Mechanochemistry and Mechanical Alloying, INCOME2022, Cagliari (Italy), June 2022.
5. 5th conference on Theory and Applications of Computational Chemistry (TACC2023), Sapporo (Japan), September 2023.

### **Presentations summary**

Since January 2015, 37 invited presentations in international conferences, and 14 invited seminars in universities and research institutes.

### **Organisation of international conferences**

Chairman of three different symposia in Tarragona, each of them with more than 50 attendees. Among the symposia, “Computational Catalysis for Sustainable Chemistry”, in June 2018, a satellite of the 16<sup>th</sup> International Congress of Quantum Chemistry (ICQC-2018)

### **Mentorship of researchers**

12 thesis supervised since 2015. Among them: Ignacio Funes-Ardoiz, associate researcher (Juan de la Cierva) at Universidad de la Rioja (Spain); Rositha Kuniyil, associate professor at IIT Palakkad (India); Shaofei Ni, associate professor at Shantou University (Guangdong, China).

6 post-doctoral students hosted since 2010. Among them: Oier Lakuntza, staff scientist at EnergiGune Gasteiz (Spain); Giuseppe Sciortino, associate professor at Universitat Autònoma de Barcelona ; Iogann Tolbatov, associate professor at Università de Padova.