

Ignacio Funes Ardoiz

Academic CV

English Version (Spanish Version below)

Address:

University of La Rioja
Department of Chemistry, Centro de Investigación en Síntesis Química (CISQ)
C/Madre de Dios, 53
Logroño, España (26006)
Teléfono: +34658459852
Email: ignacio.funesa@unirioja.es

PERSONAL INFORMATION

Date of Birth: December 19, 1991
Place of Birth: Tudela (Navarra), Spain
ID-Number: 78760217-Y
ORCID ID: 0000-0002-5843-9660
Current Position:
Humboldt postdoctoral researcher at RWTH Aachen University in the group of Prof. Schoenebeck from October, 2018.

EDUCATION

University of La Rioja (UR), Logroño, Spain
Bachelor degree in Chemistry (in Spanish)
September 2009 – June 2013
Average mark: 9.58/10; 3.71/4 (43/55 courses with honor distinction)

University Rovira i Virgili (URV) – Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain
Master of Science in Synthesis, Catalysis and Molecular Design (in English)
September 2013 – July 2014
Average mark: 9.48/10; 3.15/4 (2/8 courses with honor distinction)
Master Thesis: “*Rationalization of the Allylic Alkene Amination Mechanism with a Hypervalent Iodine(III) Reagent*”
Supervisor: Prof. Feliu Maseras

Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain
PhD in Theoretical and Computational Chemistry
October 2014 – September 2017
Calification: Excellent with distinction Cum Laude
Thesis: “*Computational Chemistry for Homogeneous Redox Catalysis*”
Supervisor: Prof. Feliu Maseras

RESEARCH EXPERIENCE

University of La Rioja (UR), Logroño, Spain

Computational photochemistry of photoswitches and carbene reactivity

2011-2013

Research group: Dr. Diego Sampedro

Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain

Computational chemistry for homogeneous redox catalysis

2013-2017

Research Group: Prof. Feliu Maseras

RWTH Aachen University, Institute of Organic Chemistry, Aachen, Germany

Computational Chemistry for Homogeneous Catalysis

01-10-2018-now

Research group: Prof. Franziska Schoenebeck

University of La Rioja (UR), Logroño, Spain

Computational photochemistry

01-10-2021-now

Independent Researcher in the Photochemistry Group of La Rioja (GRUFOR)

RESEARCH STAYS

University of Oxford, Oxford, United Kingdom

Research stay financed by Severo Ochoa Predoctoral Grant SVP-2014-068662

06/07/2015-06/10/2015

Supervisor: Prof. Robert S. Paton

University Autònoma de Barcelona, Barcelona, Spain

Research stay financed by Severo Ochoa Predoctoral Grant SVP-2014-068662

01/02/2017-28/02/2017

Supervisor: Prof. Jean-Didie Marechal

PUBLICATIONS

Total number: 31

h-index: 12 (from Google Scholar Citations on 04/03/2020)

Total citations: 512 (from Google Scholar Citations on 04/03/2020)

1- "Oxazolone-based photoswitches: Synthesis and properties"

Blanco-Lomas, M.; Funes-Ardoiz, I.; Campos, P.J.; Sampedro, D. *Eur. J. Org. Chem.* **2013**, *29*, 6611-6618.

2- "Benzylidene-oxazolones as photoswitches: Photochemistry and theoretical calculations"

Funes-Ardoiz, I.; Blanco-Lomas, M.; Campos, P.J.; Sampedro, D. *Tetrahedron* **2013**, *69*, 9766-9771.

3- "Intermolecular and regioselective access to polysubstituted benzo- and dihydrobenzo[c]azepine derivatives: Modulating the reactivity of group 6 non-heteroatom-stabilized alkynyl carbene complexes"

González, J.; Gómez, A.; Funes-Ardoiz, I.; Santamaría, J.; Sampedro, D. *Chem. Eur. J.* **2014**, *20*, 7061-7068.

4- "Computational assessment of non-heteroatom-stabilized carbene complexes reactivity: Formation of oxazine derivatives"

Funes-Ardoiz, I.; Sampedro, D. *J. Org. Chem.* **2014**, *79*, 11824-11828.

5- "On the mechanism of the Shapiro reaction: understanding the regioselectivity"

Funes-Ardoiz, I.; Sampedro, D. *RSC Adv.* **2015**, *5*, 37292-37297.

6- "Redox Non-Innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts"

Garrido-Barros, P.; Funes-Ardoiz, I.; Drouet, S.; Benet-Buchholz, J.; Maseras, F.; Llobet, A. *J. Am. Chem. Soc.* **2015**, *137*, 6758.

7- "Funcionalization of C_nH_{2n+2} Alkanes: Supercritical Carbon Dioxide Enhances the Reactivity towards Primary Carbon-Hydrogen Bonds"

Gava, R.; Olmos, A.; Noverges, B.; Varea, T.; Funes-Ardoiz, I.; Belderrain, T.R.; Caballero, A.; Maseras, F.; Asensio, G.; Pérez, P.J.. *ChemCatChem.* **2015**, *7*, 3254.

8- “Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle”

Funes-Ardoiz, I.; Maseras, F. *Angew. Chem. Int. Ed.* **2016**, *55*, 2764.

9- “Understanding the Mechanism of the Divergent Reactivity of Non-Heteroatom-Stabilized Chromium Carbene Complexes with Furfural Imines: Formation of Benzofurans and Azetines”

Funes-Ardoiz, I.; González, J.; Santamaría, J.; Sampedro, D. *J. Org. Chem.* **2016**, *81*, 1565-1570.

10- “DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes”

Funes-Ardoiz, I.; Sameera, W. M. C.; Romero, R. M.; Martínez, C.; Souto, J. A.; Sampedro, D.; Muñiz, K.; Maseras, F. *Chem. Eur. J.* **2016**, *22*, 7545-7553.

11- “Single Electron Transfer Steps in Water Oxidation Catalysis. Redefining the Mechanistic Scenario”

Funes-Ardoiz, I.; Garrido-Barros, P.; Llobet, A.; Maseras, F. *ACS Catal.* **2017**, *7*, 1712-1719.

12- “Rational Design and Synthesis of Efficient Sunscreens To Boost the Solar Protection Factor”

Losantos, R.; Funes-Ardoiz, I.; Aguilera, J.; Herrera-Ceballos, E.; García-Iriepa, C.; Campos, P. J.; Sampedro, D. *Angew. Chem. Int. Ed.* **2017**, *56*, 2632-2635.

(Highlighted in *C&EN*, *The Medical News*, *ChemistryViews*, *Forbes*, *Phys.org* and *EurekAlert!*)

13- “Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with $[\text{Ni}(\text{PMe}_n\text{Ph}_{(3-n)})_4]$ ”

Funes-Ardoiz, I.; Nelson, D. J.; Maseras, F. *Chem. Eur. J.* **2017**, *23*, 16728-16733.

14- “Oxidative Coupling Mechanisms: Current State of Understanding”

Funes-Ardoiz, I.; Maseras, F. *ACS Catal.* **2018**, *8*, 1161-1172. (Selected as ACS Editors' Choice)

15- "Enantioselective Synthesis of Aminodiols by Sequential Rh-Catalysed Oxyamination/Kinetic Resolution. Expanding the Substrate Scope of Amidine-Based Catalysis"

Guasch, J.; Giménez, I.; Funes-Ardoiz, I.; Matheu, I.; Maseras, F.; Castellón, S.; Díaz, Y.; Bernús, M. *Chem. Eur. J.* **2018**, *24*, 4635-4642.

16- "Elucidating the Mechanism of Aryl Aminations Mediated by NHC-Supported Nickel Complexes: Evidence for a Nonradical Ni(0)/Ni(II) Pathway"

Rull, S. G.; Funes-Ardoiz, I.; Maya, C.; Maseras, F.; Fructos, M. R.; Belderrain, T. R.; Nicasio, M. C. *ACS Catal.* **2018**, *8*, 3733-3742.

17- "Computational Characterization of the Mechanism for the Oxidative Coupling of Benzoic Acid and Alkynes by Rhodium/Copper and Rhodium/Silver Systems"

Funes-Ardoiz, I. (corresponding author); Maseras, F. *Chem. Eur. J.* **2018**, *24*, 12383-12388. (*Special Issue: Young Chemists*).

18- "Accelerated Ru-Cu Trinuclear Cooperative C-H Bond Functionalization of Carbazoles: a Kinetic and Computational Investigation"

Jones, A.; Rank, C.; Becker, Y.; Malchau, C.; Funes-Ardoiz, I.; Maseras, F.; Patureau, F. W. *Chem. Eur. J.* **2018**, *24*, 15178-15184.

19- "Unexpected [4+ 2] Cycloaddition through Chromium Non-Heteroatom-Stabilized Alkynyl Carbene Complexes: Regioselective Access to Substituted 6-Azaindoles"

Gómez, A.; Funes-Ardoiz, I.; Sampedro, D.; Santamaría, J. *Org. Lett.* **2018**, *20*, 4099-4102.

20- "Palladium-Catalyzed Aerobic Homocoupling of Alkynes: Full Mechanistic Characterization of a More Complex Oxidase-type Behavior"

Toledo, A.; Funes-Ardoiz, I.; Maseras, F.; Albeniz, A. C. *ACS Catal.* **2018**, *8*, 7485-7506.

21- “Catalytic Enantio- and Diastereoselective Mannich Addition of TosMIC to Ketimines”

Franchino, A.; Chapman, J.; Funes-Ardoiz, I.; Paton, R. S.; Dixon, D. J. *Chem. Eur. J.* **2018**, *24*, 17660-17664.

22- “GARLEEK: Adding and Extra Flavor to ONIOM”

Rodríguez-Guerra Pedregal, J.; Funes-Ardoiz, I.; Sciortino, G.; Sánchez-Aparicio, J.-E.; Ujaque, G.; Lledós, A.; Maréchal, J.-D.; Maseras, F. *J. Comp. Chem.* **2019**, *40*, 381-386. (Special Issue: Memorial Festschrift for Keiji Morokuma)

23- “On the Use of Thermodynamic Cycles for the Calculation of Standard Potentials for the Oxidation of Solid Metals in Solution”

Funes-Ardoiz, I.; Maseras, F. *ChemPhysChem* **2019**, *20*, 159-162.

24- “Computational Characterization of Single-Electron Transfer Steps in Water Oxidation”

De Aguirre, A.; Funes-Ardoiz, I.; Maseras, F. *Inorganics* **2019**, *7*, 32.

25- “Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study”

De Aguirre, A.; Funes-Ardoiz, I.; Maseras, F. *Angew. Chem. Int. Ed.* **2019**, *58*, 3898-3902.

26- “Copper-Catalyzed N–F Bond Activation for Uniform Intramolecular C–H Amination Yielding Pyrrolidines and Piperidines”

Bafaluy, D.; Muñoz-Molina, J. M.; Funes-Ardoiz, I.; Herold, S.; de Aguirre, A.J.; Zhang, H.; Maseras, F.; Belderrain, T.R.; Pérez, P.J.; Muñiz, K. *Angew. Chem. Int. Ed.* **2019**, *58*, 8912-8916.

- 27- “The Role of Electron-Donor Substituents in the Family of OPBAN-Cu Water Oxidation Catalysts: Effect on the Degradation Pathways and Efficiency”
De Aguirre, A.; Garrido-Barros, P.; Funes-Ardoiz, I. (as corresponding autor); Maseras, F. *Eur. J. Inor. Chem.* **2019**, 2109-2114.
- 28- “Enantioselective Synthesis of 3-Heterosubstituted-2-amino-1-ols by Sequential Metal-Free Diene Aziridination/Kinetic Resolution”
Giménez-Nueno, I.; Guasch, J.; Funes-Ardoiz, I.; Maseras, F.; Matheu, M.I.; Castellón, S.; Díaz, Y. *Chem. Eur. J.* **2019**, *25*, 12628-12635. (Hot paper)
- 29- “Orthogonal Nanoparticle Catalysis with Organogermanes”
Fricke, C.; Sherborne, G. J.; Funes-Ardoiz, I.; Senol, E.; Guven, S.; Schoenebeck, F. *Angew. Chem. Int. Ed.* **2019**, *58*, 17788-17795.
- 30- “Stability of Hierarchically Formed Titanium(IV) Tris(catecholate ester) Helicates with Cyclohexyl Substituents in DMSO”
Schlottmann, M.; Van Craen, D.; Baums, J.; Funes-Ardoiz, I.; Wiederhold, C.; Oppel, I. M.; Albrecht, M. *Inorg. Chem.* **2020**, *59*, 1758-1762.
- 31- “Selective Ortho Functionalization of Adamantylarenes enabled by Dispersion and an Air-Stable Pd(I) Dimer”
Kalvet, I.; Deckers, C.; Funes-Ardoiz, I.; Magnin, G.; Sperger, T.; Kremer, M.; Schoenebeck, F. *Angew. Chem. Int. Ed.* **2020**, *132*, 7795-7799.
- 32- “GoodVibes: automated thermochemistry for heterogeneous computational chemistry data”
Luchini, G.; Alegre-Requena, J. V.; Funes-Ardoiz, I.; Paton, R. S. *F1000Research*, **2020**, *9*, 291.
- 33- “Modular and Selective Arylation of Aryl Germanes (C–GeEt₃) over C–Bpin, C–SiR₃ and Halogens Enabled by Light-Activated Gold Catalysis”
Sherborne, G. J.; Gevondian, A. G.; Funes-Ardoiz, I., Dahiya, A.; Fricke, C.; Schoenebeck, F. *Angew. Chem. Int. Ed.* **2020**, *59*, 15543-15548.

- 34- “Work-hardening Photopolymer from Renewable Photoactive 3, 3’-(2, 5-Furandiyl) bisacrylic Acid”
Lie, T.; Pellis, A.; Funes-Ardoiz, I.; Sampedro, D.; Macquarrie, D. J.; Farmer, T. J. *ChemSusChem*. **2020**, *13*, 4140.
- 35- “Established and emerging computational tools to study homogeneous catalysis—From quantum mechanics to machine learning”
Funes-Ardoiz, I.; Schoenebeck, F. *Chem*. **2020**, *6*, 1904-1913.
- 36- “Photocontrolled Cobalt Catalysis for Selective Hydroboration of α , β -Unsaturated Ketones”
Beltran, F.; Bergamaschi, E.; Funes-Ardoiz, I.; Teskey, C. J. *Angew. Chem. Int. Ed.* **2020**, *59*, 21176-21182.
- 37- “Consecutive Ligand-Based Electron Transfer in New Molecular Copper-Based Water Oxidation Catalysts”
Gil-Sepulcre, M.; Barrido-Barros, P.; Oldengott, J.; Funes-Ardoiz, I.; Bofill, R.; Benet-Buchholz, J.; Llobet, A. *Angew. Chem. Int. Ed.* **2021**, *60*, 18639-18644.
- 37- “Consecutive Ligand-Based Electron Transfer in New Molecular Copper-Based Water Oxidation Catalysts”
Gil-Sepulcre, M.; Barrido-Barros, P.; Oldengott, J.; Funes-Ardoiz, I.; Bofill, R.; Benet-Buchholz, J.; Llobet, A. *Angew. Chem. Int. Ed.* **2021**, *60*, 18639-18644.
- 38- “Dual Photoredox/Cobaloxime Catalysis for Cross-Dehydrogenative α -Heteroarylation of Amines”
Bergamaschi, E.; Weike, C.; Mayerhofer, V. J.; Funes-Ardoiz, I. (corresponding author); Teskey, C. J. *Org. Lett.* **2021**, *23*, 5378-5382.
- 39- “Hydroalkylation of Unactivated Olefins via Visible-Light-Driven Dual Hydrogen Atom Transfer Catalysis”

Lei, G.; Xu, M.; Chang, R.; Funes-Ardoiz, I. (corresponding author); Ye, J. *J. Am. Chem. Soc.* **2021**, *143*, 11251-11261.

BOOK CHAPTER

1- Chapter title: “Water as an Oxygen Source for Oxidation Reactions” in book “Science of Synthesis: Catalytic Oxidation in Organic Synthesis” (Ed. Prof. Kilian Muñiz, Editorial: Georg Thieme Verlag KG, 2017).

Authors: Garrido-Barros, P.; Funes-Ardoiz, I.; Farràs, P.; Gimbert-Suriñach, C.; Maseras, F.; Llobet, A.

2- Chapter title: “Introduction to the Mechanistic Scenario in Water Oxidation Catalysis by Transition Metal Complexes” (Ed. James C. Taylor, Editorial: Nova Science Publishers Inc., New York, 2020). ISBN: 978-1-53618-734-2

Autores: Garrido-Barros, P.; Funes-Ardoiz, I. (Corresponding author)

PATENTS

1-Title: “Compuestos fotoprotectores análogos de MMA, procedimiento de síntesis y composición que comprende los mismos”. Inventors: Diego Sampedro, Raúl Losantos, Ignacio Funes.

Patent code: ES-2550374

2-Title: “Analogues of mycosporine-like amino acid and use thereof as sunscreens”. Applicant: BASF SE. Inventors: Diego Sampedro, Raúl Losantos, Ignacio Funes-Ardoiz, Thomas Ehlis, Jochen Giesinger, Julie Grume-Lard.

Patent code: WO 2021/148426 A1

DEVELOPED SOFTWARE

1- **GoodVibes:** Python program to compute thermochemical data from one or a series of electronic structure calculations, including quasi-harmonic corrections

Developed by: Paton, R.S.; Funes-Ardoiz, I.; Luchini, G.; Alegre-Requena, J.V.; Guan, Y.; Rodriguez-Guerra, J.

Citations: 37. DOI: 10.5281/zenodo.3346166.

Free download available from: <https://github.com/bobbypaton/GoodVibes>

2- **GARLEEK**: Python program to do QM/MM (ONIOM) calculations using Gaussian software for QM part and Tinker for MM part.

Developed by: Rodríguez-Guerra Pedregal, J.; Funes-Ardoiz, I.; Sciortino, G.; Sánchez-Aparicio, J.-E.; Ujaque, G.; Lledós, A.; Maréchal, J.-D.; Maseras, F.

Citations: 2. Cite as: *J. Comp. Chem.* **2019**, *40*, 381-386.

Free download available from: <https://github.com/insilichem/garleek>

2- **EasyMECP**: Python program to calculate Minimum Energy Crossing Points (MECP) in Gaussian software

Developed by: Rodríguez-Guerra Pedregal, J.; Funes-Ardoiz, I.; Maseras, F.

Free download available from: <https://github.com/jaimergp/easymecp>

ORAL COMMUNICATIONS IN CONFERENCES

1- XII Simposio de Investigadores Jóvenes RSEQ-Sigma Aldrich, Barcelona (JIQ-RSEQ), Spain. 3rd -6th November, 2015.

“A Mechanistic Approach to the Overpotential Control in Cu-Based Water Oxidation Catalysis”

Funes-Ardoiz, I.

2- IX Trobada de Joves Investigadors del Països Catalans, Perpignan (SCQ-UPVD), France. 3rd -5th February, 2016.

“El Mecanisme de Formació de l’Enllaç O-O en una Nova Família de Catalitzadors de Coure per a Rumpura d’Aigua/ The Mechanism of the O-O Bond Formation in a New Family of Copper Catalist for Water Splitting”

Funes-Ardoiz, I.

3- IX International School on Organometallic Chemistry “Marcial Moreno Mañas”, Donostia-San Sebastián (UPV-EHU), Spain. 6th -8th, July, 2016.

“A Computational Study on the Role of Copper Diacetate in Oxidative Coupling Reactions”

Funes-Ardoiz, I.

4- 6th EuCheMS Chemistry Congress, Seville (FIBES), Spain. 11th -15th, September, 2016.

“The Cooperative Effect of Transition Metal Catalysts in the Oxidative Cross-Couplings. A DFT Mechanistic Study” (another oral communication in the special symposium of the European Young Chemistry Awards (EYCA), as a finalist of the competition)

Funes-Ardoiz, I.

5- XIII Simposio de Investigadores Jóvenes de la Real Sociedad Española de Química, Logroño (Unirioja), Spain. 8th -11th, November, 2016.

“Is One Metal Enough? The Role of Copper Acetate in Oxidative Coupling”

Funes-Ardoiz, I.

6- V COST-CARISMA 2017 Meeting. Lisbon (Sana Malhoa Hotel), Portugal. 6th -8th March, 2017.

“The Single Electron Transfer Mechanism for Oxygen-Oxygen Bond Formation in Copper-Based Water Oxidation Catalysis”.

Funes-Ardoiz, I.; Garrido-Barros, P.; Llobet, A.; Maseras, F.

7- BIST PhD ICIQ Meeting. Tarragona (ICIQ), Spain. 19th April, 2017.

“Computational Chemistry at ICIQ”. (Invited speaker)

Funes-Ardoiz, I.

8- XXXVI Reunión BIENAL de la RSEQ. Sitges (Hotel Melia), Spain. 25th-29th June, 2017.

“Single Electron Transfer-Water Nucleophilic Attack Mechanism in Water Oxidation reaction”.

Funes-Ardoiz, I., Garrido-Barros, P.; Llobet, A.; Maseras, F.

9- XXXVI Reunión BIENAL de la RSEQ. Sitges (Hotel Melia), Spain. 25th-29th June, 2017.

“Divulgar Durante el Doctorado, ¿Misión Imposible?”

Funes-Ardoiz, I., Garrido-Barros, P.; Maseras, F.

10- International Conference of Computational Methods in Sciences and Engineering 2018 (ICCMSE 2018), The MET Hotel, Thessaloniki, Greece. 14th-18th March 2018.

“Computational Characterization on the Active Role of the Oxidant in Oxidative Coupling Reactions”. (Invited talk)

Funes-Ardoiz, I.

11- Girona Seminar: Predictive Catalysis, Transition-Metal Reactivity by Design, Girona, Spain. 3th-6th April, 2018.

“Understanding the Active Role of the Oxidant in the Oxidative Coupling of Benzoic Acid and Alkyne”.

Funes-Ardoiz, I.

12- European Colloquium on Inorganic Reaction Mechanisms 2018, Barcelona, Spain. 8th-11th July, 2018.

Contributed talk: “Exploring the Mechanism of Ru-Cu Cooperative Catalysis in the Oxidative Homocoupling of Carbazoles”.

Funes-Ardoiz, I.

13- Gordon Research Seminar on Green Chemistry 2018, Rey Don Jaime Grand Hotel in Castelldefels, Spain. 28th-29th July, 2018; Gordon Research Conference on Green Chemistry 2018, Rey Don Jaime Grand Hotel in Castelldefels, Spain. 29th July-3rd August, 2018.

Contributed talk (GRS) and poster (GRC): “Computational Insight into the Single Electron Transfer-Water Nucleophilic Attack Mechanism in Copper based Water Oxidation Catalysis”.

Funes-Ardoiz, I.

AWARDS

1- Catalysis Science and Technology Talk Award in Girona Seminar 2018.

2- 2017 Josep Castells Award from the Spanish Royal Chemistry Society.

3- 1st Price and special prize of the public in the contest: “Vols saber què investigo? (2015)” with the monologue “Rompamos el agua (splitting the water)” organized by the Universitat Rovira i Virgili. Video available on:

https://www.youtube.com/watch?v=S61Gzxx0W08&list=PL8yyYJSAXdwluigrH_bTNw9AXGJi0jao

4- Winner of the scientific contest “I’m a scientist, get me out of here” (Spanish edition), November 2016. In the environment zone. Profile available at:

<http://ambiente.somoscientificos.es/profile/ignaciofunes/>

5- 2nd Place in Falling Walls Lab Barcelona 2017. 12th September 2017.

6- Silver medal in Spanish chemistry Olympiad, 2009.

COMPETITIVE GRANTS

1- Fellowship “Iniciación a la Investigación (Introduction to research)” under the supervision of Dr. Diego Sampedro in University of La Rioja. 1/12/2011 to 30/06/2012.

2- ICIQ Summer Fellowship under the supervision of Prof. Feliu Maseras. Institute of Chemical Research of Catalonia. Summer 2012 (3 months).

3- Grant for Master studies (“Ayuda de estudio del Institut Català d’Investigació Química”) in the Institute of Chemical Research of Catalonia under the supervision of Prof. Feliu Maseras. 2013-2014

4- Predoctoral training grant for Centres/Units of Excellence “Severo Ochoa” (Call 2014). Predoctoral researcher reference: SVP-2014-068662).

5- Humboldt postdoctoral researcher grant (24 months) in RWTH Aachen University (Germany).

ACADEMIC HABILITATION

- 1- Spanish ministry “Ministerio de educación, cultura y deporte” accreditation as “Profesor Ayudante Doctor (equivalent to Assistant Professor)”. May, 2018.
- 2- Spanish ministry “Ministerio de educación, cultura y deporte” accreditation as “Profesor Contratado Doctor (equivalent to Associate Professor)”. December, 2018.

TEACHING EXPERIENCE

1- Teaching assistance in “Angewandte Computer Chemie (Applied computational chemistry)” master course. 3 ECTS credits. Universidad RWTH Aachen. 2019-2020.

2- Master internship supervision at RWTH University:

Name of student: Julian Hüffel

Matrkl. number: 380507

Start and ending date: Start: 13.03.2019; End: 10.05.2019

type of project: Computational characterization of cross-coupling organic reactions

length of project: 30 days + 2 weeks buffer

due date of thesis/report: 03.06.2019

Name of student: Clara Nussbaumer

Matrkl. number: 344098

Start and ending date: Start: 06.05.19; End 28.06.19

Type of project: Computational study of copper-catalyzed C-C bond cleavage.

Length of project: approx. 2 months

Due date of thesis/report: 12.07.19

Name of student: Hendrik Simon

Matrkl. number: Visiting student from Technische Universität Berlin.

Start and ending date: Start: 07.10.19; End 07.12.19

Type of project: Computational study of homogeneous Pd nanocluster catalysis of Heck reaction.

Length of project: approx. 2 months

Due date of thesis/report: 07.12.19

Name of student: Sander Folkerts

Matrkl. number: 355785

Start and ending date: Start: 14.11.19; End 23.01.2020

Type of project: Computational study of SN2 reaction for machine learning applications

Length of project: approx. 2 months

Due date of thesis/report: 23.01.2020

3- Master thesis supervision at RWTH University (ongoing):

Name of student: Julian Hüffel

Matrkl. number: 380507

Start and ending date: Start: 21.10.2019; End: 21.04.2020

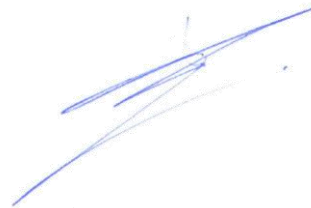
type of project: Applied Machine Learning in Computational Chemistry
length of project: 6 months
due date of thesis/report: 21.04.2020

OUTREACH ACTIVITIES

- 1- **Participation at the Scientific Monologue Competition “Vols saber què investigo? (2015)”** with the monologue “Romparamos el agua (splitting the water)”. November, 2015. Organized by Unitat de Comunicació de la Ciència of the URV university.
- 2- **Scientific Monologues at the Institute Martí i Franquès.** 22th April, 2016. Organized by Unitat de Comunicació de la Ciència of the URV university.
- 3- **Festa de la Ciència Barcelona 2016-Talk “Trenquem l’aigua” and workshop “Catàlisi Exprès”** 18-19th Juny, 2016. Organized by Barcelona Ciència and Ajuntament de Barcelona at the Parc de la Ciutadella. Video online: <https://www.youtube.com/watch?v=6Cgc0pw4b6k>
- 4- **Participation at the Scientific Monologue Competition “Vols saber què investigo? (2016) as jury**
- 5- **Participation in the activity “Dia de la Ciència a les Escoles” at the INS Martí l’Humà in Montblanc with the talk “¿Se puede ser químico sin bata de laboratorio?”** 16th November, 2016. Organized by Unitat de Comunicació de la Ciència of the URV university.
- 6- **Participation in the contest “I’m a scientist, get me out of here” (Spanish edition),** November 2016. In the environment zone.
- 7- **Invited talk entitles “Mi experiencia investigadora” at the high school IES Benjamín de Tudela in Tudela** 7th December, 2016. Organized by IES Benjamín de Tudela.
- 8- **Participation in “Fira Taster de Ciència 2017” with a monologue entitle “Fotoprotége”** at the Centro de Lectura de Reus 17th May, 2017. Organized by Centre de Recursos pedagògics Baix Camp.
- 9- **Invited talk in the symposium “Seguim Bojos per la Química” which is entitled “Se puede ser químico sin bata de laboratorio?”**, 7th July, 2017. ICIQ, Tarragona.
- 10- **Participation in “Falling Walls Lab Barcelona” with the talk “Breaking the Wall of Energy Production”**, 12th September, 2017. UPF, Barcelona.
- 1- **Participation in the activity “Dia de la Ciència a les Escoles” at the INS Joan Puig i Ferrater at La Selva del Camp with the talk “¿Se puede ser químico sin bata de laboratorio?”** 15th November, 2017. Organized by “Fundació Catalana per a la Recerca i la Innovació”.

12- Participation in the Pint of Science Festival 2018 (Tarragona edition) at Vinateria Clot Martell with the talk “Imitemos a las plantas”. 14th May, 2018.
Organized by Pint of Science Spain.

Signature:

A handwritten signature in blue ink, consisting of several overlapping, sweeping lines that form a stylized, abstract shape.

Dr. Ignacio Funes Ardoiz
Aachen, 04/03/2020

Ignacio Funes Ardoiz

CV Académico

Versión en Castellano

Dirección:

University of La Rioja
Department of Chemistry, Centro de Investigación en Síntesis Química (CISQ)
C/Madre de Dios, 53
Logroño, España (26006)
Teléfono: +34658459852
Email: ignacio.funesa@unirioja.es

INFORMACIÓN PERSONAL

Fecha de Nacimiento: 19 de diciembre, 1991
Lugar de Nacimiento: Tudela (Navarra), España
DNI: 78760217-Y
ORCID ID: 0000-0002-5843-9660
Posición actual:
Investigador Juan de la Cierva en el Grupo de Fotoquímica de la Universidad de La Rioja

EDUCACION

Universidad of La Rioja (UR), Logroño, España

Licenciatura en Química

Septiembre 2009 – Junio 2013

Nota media de expediente: 9.58/10; 3.71/4 (43/55 asignaturas con matrícula de honor)

Universidad Rovira i Virgili (URV) – Instituto Catalán de Investigación Química (ICIQ), Tarragona, España

Master en “Synthesis, Catalysis and Molecular Design” (en inglés)

Septiembre 2013 – Julio 2014

Nota media de expediente: 9.48/10; 3.15/4 (2/8 asignaturas con matrícula de honor)

Master Thesis: “*Rationalization of the Allylic Alkene Amination Mechanism with a Hypervalent Iodine(III) Reagent*”

Supervisor: Prof. Feliu Maseras

Instituto Catalán de Investigación Química (ICIQ), Tarragona, España

PhD en “Ciencia y Tecnología Química” (especializado en química teórica y computacional)

Octubre 2014 – Septiembre 2017

Calificación: Excellent with distinction Cum Laude

Título de tesis: “*Computational Chemistry for Homogeneous Redox Catalysis*”

Supervisor: Prof. Feliu Maseras

EXPERIENCIA INVESTIGADORA

University of La Rioja (UR), Logroño, Spain

Computational photochemistry of photoswitches and carbene reactivity

2011-2013

Grupo de Investigación: Dr. Diego Sampedro

Institute of Chemical Research of Catalonia (ICIQ), Tarragona, Spain

Computational chemistry for homogeneous redox catalysis

2013–2017

Grupo de Investigación: Prof. Feliu Maseras

RWTH Aachen University, Institute of Organic Chemistry, Aachen, Germany

Computational Chemistry for Homogeneous Catalysis

01-10-2018-30-09-2020

Grupo de Investigación:: Prof. Franziska Schoenebeck

University of La Rioja (UR), Logroño, Spain

Computational photochemistry

01-10-2021-now

Investigador independiente en el Grupo de Fotoquímica de La Rioja (GRUFOR)

ESTANCIAS DE INVESTIGACIÓN

Universidad de Oxford, Oxford, Reino Unido

Estancia de investigación financiada por la ayuda predoctoral de excelencia

Severo Ochoa SVP-2014-068662

06/07/2015-06/10/2015

Supervisor: Prof. Robert S. Paton

Universidad Autónoma de Barcelona, Barcelona, España

Estancia de investigación financiada por la ayuda predoctoral de excelencia

Severo Ochoa SVP-2014-068662

01/02/2017-28/02/2017

Supervisor: Prof. Jean-Didie Marechal

PUBLICACIONES

Número total: 40

h-index: 16 (Fuente: Google Scholar Citations on 10/09/2021)

Citas totales: 907 (Fuente: Google Scholar Citations on 10/09/2021)

1- "Oxazolone-based photoswitches: Synthesis and properties"

Blanco-Lomas, M.; Funes-Ardoiz, I.; Campos, P.J.; Sampedro, D. *Eur. J. Org. Chem.* **2013**, 29, 6611-6618.

2- "Benzylidene-oxazolones as photoswitches: Photochemistry and theoretical calculations"

Funes-Ardoiz, I.; Blanco-Lomas, M.; Campos, P.J.; Sampedro, D. *Tetrahedron* **2013**, 69, 9766-9771.

3- "Intermolecular and regioselective access to polysubstituted benzo- and dihydrobenzo[c]azepine derivatives: Modulating the reactivity of group 6 non-heteroatom-stabilized alkynyl carbene complexes"

González, J.; Gómez, A.; Funes-Ardoiz, I.; Santamaría, J.; Sampedro, D. *Chem. Eur. J.* **2014**, 20, 7061-7068.

4- "Computational assessment of non-heteroatom-stabilized carbene complexes reactivity: Formation of oxazine derivatives"

Funes-Ardoiz, I.; Sampedro, D. *J. Org. Chem.* **2014**, 79, 11824-11828.

5- "On the mechanism of the Shapiro reaction: understanding the regioselectivity"

Funes-Ardoiz, I.; Sampedro, D. *RSC Adv.* **2015**, 5, 37292-37297.

6- "Redox Non-Innocent Ligand Controls Water Oxidation Overpotential in a New Family of Mononuclear Cu-Based Efficient Catalysts"

Garrido-Barros, P.; Funes-Ardoiz, I.; Drouet, S.; Benet-Buchholz, J.; Maseras, F.; Llobet, A. *J. Am. Chem. Soc.* **2015**, 137, 6758-6761.

7- "Funcionalization of C_nH_{2n+2} Alkanes: Supercritical Carbon Dioxide Enhances the Reactivity towards Primary Carbon-Hydrogen Bonds"

Gava, R.; Olmos, A.; Noverges, B.; Varea, T.; Funes-Ardoiz, I.; Belderrain, T.R.; Caballero, A.; Maseras, F.; Asensio, G.; Pérez, P.J.. *ChemCatChem.* **2015**, 7, 3254-3260.

8- “Cooperative Reductive Elimination: The Missing Piece in the Oxidative-Coupling Mechanistic Puzzle”

Funes-Ardoiz, I.; Maseras, F. *Angew. Chem. Int. Ed.* **2016**, *55*, 2764.

9- “Understanding the Mechanism of the Divergent Reactivity of Non-Heteroatom-Stabilized Chromium Carbene Complexes with Furfural Imines: Formation of Benzofurans and Azetines”

Funes-Ardoiz, I.; González, J.; Santamaría, J.; Sampedro, D. *J. Org. Chem.* **2016**, *81*, 1565-1570.

10- “DFT Rationalization of the Diverse Outcomes of the Iodine(III)-Mediated Oxidative Amination of Alkenes”

Funes-Ardoiz, I.; Sameera, W. M. C.; Romero, R. M.; Martínez, C.; Souto, J. A.; Sampedro, D.; Muñiz, K.; Maseras, F. *Chem. Eur. J.* **2016**, *22*, 7545-7553.

11- “Single Electron Transfer Steps in Water Oxidation Catalysis. Redefining the Mechanistic Scenario”

Funes-Ardoiz, I.; Garrido-Barros, P.; Llobet, A.; Maseras, F. *ACS Catal.* **2017**, *7*, 1712-1719.

12- “Rational Design and Synthesis of Efficient Sunscreens To Boost the Solar Protection Factor”

Losantos, R.; Funes-Ardoiz, I.; Aguilera, J.; Herrera-Ceballos, E.; García-Iriepa, C.; Campos, P. J.; Sampedro, D. *Angew. Chem. Int. Ed.* **2017**, *56*, 2632-2635.

(Highlighted in *C&EN*, *The Medical News*, *ChemistryViews*, *Forbes*, *Phys.org* and *EurekAlert!*)

13- “Halide Abstraction Competes with Oxidative Addition in the Reactions of Aryl Halides with $[\text{Ni}(\text{PMe}_n\text{Ph}_{(3-n)})_4]$ ”

Funes-Ardoiz, I.; Nelson, D. J.; Maseras, F. *Chem. Eur. J.* **2017**, *23*, 16728-16733.

14- “Oxidative Coupling Mechanisms: Current State of Understanding”

Funes-Ardoiz, I.; Maseras, F. *ACS Catal.* **2018**, *8*, 1161-1172. (Selected as ACS Editors' Choice)

15- "Enantioselective Synthesis of Aminodiols by Sequential Rh-Catalysed Oxyamination/Kinetic Resolution. Expanding the Substrate Scope of Amidine-Based Catalysis"

Guasch, J.; Giménez, I.; Funes-Ardoiz, I.; Matheu, I.; Maseras, F.; Castellón, S.; Díaz, Y.; Bernús, M. *Chem. Eur. J.* **2018**, *24*, 4635-4642.

16- "Elucidating the Mechanism of Aryl Aminations Mediated by NHC-Supported Nickel Complexes: Evidence for a Nonradical Ni(0)/Ni(II) Pathway"

Rull, S. G.; Funes-Ardoiz, I.; Maya, C.; Maseras, F.; Fructos, M. R.; Belderrain, T. R.; Nicasio, M. C. *ACS Catal.* **2018**, *8*, 3733-3742.

17- "Computational Characterization of the Mechanism for the Oxidative Coupling of Benzoic Acid and Alkynes by Rhodium/Copper and Rhodium/Silver Systems"

Funes-Ardoiz, I. (corresponding author); Maseras, F. *Chem. Eur. J.* **2018**, *24*, 12383-12388. (*Special Issue: Young Chemists*).

18- "Accelerated Ru-Cu Trinuclear Cooperative C-H Bond Functionalization of Carbazoles: a Kinetic and Computational Investigation"

Jones, A.; Rank, C.; Becker, Y.; Malchau, C.; Funes-Ardoiz, I.; Maseras, F.; Patureau, F. W. *Chem. Eur. J.* **2018**, *24*, 15178-15184.

19- "Unexpected [4+ 2] Cycloaddition through Chromium Non-Heteroatom-Stabilized Alkynyl Carbene Complexes: Regioselective Access to Substituted 6-Azaindoles"

Gómez, A.; Funes-Ardoiz, I.; Sampedro, D.; Santamaría, J. *Org. Lett.* **2018**, *20*, 4099-4102.

20- "Palladium-Catalyzed Aerobic Homocoupling of Alkynes: Full Mechanistic Characterization of a More Complex Oxidase-type Behavior"

Toledo, A.; Funes-Ardoiz, I.; Maseras, F.; Albeniz, A. C. *ACS Catal.* **2018**, *8*, 7485-7506.

21- “Catalytic Enantio- and Diastereoselective Mannich Addition of TosMIC to Ketimines”

Franchino, A.; Chapman, J.; Funes-Ardoiz, I.; Paton, R. S.; Dixon, D. J. *Chem. Eur. J.* **2018**, *24*, 17660-17664.

22- “GARLEEK: Adding and Extra Flavor to ONIOM”

Rodríguez-Guerra Pedregal, J.; Funes-Ardoiz, I.; Sciortino, G.; Sánchez-Aparicio, J.-E.; Ujaque, G.; Lledós, A.; Maréchal, J.-D.; Maseras, F. *J. Comp. Chem.* **2019**, *40*, 381-386. (Special Issue: Memorial Festschrift for Keiji Morokuma)

23- “On the Use of Thermodynamic Cycles for the Calculation of Standard Potentials for the Oxidation of Solid Metals in Solution”

Funes-Ardoiz, I.; Maseras, F. *ChemPhysChem* **2019**, *20*, 159-162.

24- “Computational Characterization of Single-Electron Transfer Steps in Water Oxidation”

De Aguirre, A.; Funes-Ardoiz, I.; Maseras, F. *Inorganics* **2019**, *7*, 32.

25- “Four Oxidation States in a Single Photoredox Nickel-Based Catalytic Cycle: A Computational Study”

De Aguirre, A.; Funes-Ardoiz, I.; Maseras, F. *Angew. Chem. Int. Ed.* **2019**, *58*, 3898-3902.

26- “Copper-Catalyzed N–F Bond Activation for Uniform Intramolecular C–H Amination Yielding Pyrrolidines and Piperidines”

Bafaluy, D.; Muñoz-Molina, J. M.; Funes-Ardoiz, I.; Herold, S.; de Aguirre, A.J.; Zhang, H.; Maseras, F.; Belderrain, T.R.; Pérez, P.J.; Muñiz, K. *Angew. Chem. Int. Ed.* **2019**, *58*, 8912-8916.

- 27- “The Role of Electron-Donor Substituents in the Family of OPBAN-Cu Water Oxidation Catalysts: Effect on the Degradation Pathways and Efficiency”
De Aguirre, A.; Garrido-Barros, P.; Funes-Ardoiz, I. (as corresponding autor); Maseras, F. *Eur. J. Inor. Chem.* **2019**, 2109-2114.
- 28- “Enantioselective Synthesis of 3-Heterosubstituted-2-amino-1-ols by Sequential Metal-Free Diene Aziridination/Kinetic Resolution”
Giménez-Nueno, I.; Guasch, J.; Funes-Ardoiz, I.; Maseras, F.; Matheu, M.I.; Castellón, S.; Díaz, Y. *Chem. Eur. J.* **2019**, *25*, 12628-12635. (Hot paper)
- 29- “Orthogonal Nanoparticle Catalysis with Organogermanes”
Fricke, C.; Sherborne, G. J.; Funes-Ardoiz, I.; Senol, E.; Guven, S.; Schoenebeck, F. *Angew. Chem. Int. Ed.* **2019**, *58*, 17788-17795.
- 30- “Stability of Hierarchically Formed Titanium(IV) Tris(catecholate ester) Helicates with Cyclohexyl Substituents in DMSO”
Schlottmann, M.; Van Craen, D.; Baums, J.; Funes-Ardoiz, I.; Wiederhold, C.; Oppel, I. M.; Albrecht, M. *Inorg. Chem.* **2020**, *59*, 1758-1762.
- 31- “Selective Ortho Functionalization of Adamantylarenes enabled by Dispersion and an Air-Stable Pd(I) Dimer”
Kalvet, I.; Deckers, C.; Funes-Ardoiz, I.; Magnin, G.; Sperger, T.; Kremer, M.; Schoenebeck, F. *Angew. Chem. Int. Ed.* **2020**, *132*, 7795-7799.
- 32- “GoodVibes: automated thermochemistry for heterogeneous computational chemistry data”
Luchini, G.; Alegre-Requena, J. V.; Funes-Ardoiz, I.; Paton, R. S. *F1000Research*, **2020**, *9*, 291.
- 33- “Modular and Selective Arylation of Aryl Germanes (C–GeEt₃) over C–Bpin, C–SiR₃ and Halogens Enabled by Light-Activated Gold Catalysis”
Sherborne, G. J.; Gevondian, A. G.; Funes-Ardoiz, I.; Dahiya, A.; Fricke, C.; Schoenebeck, F. *Angew. Chem. Int. Ed.* **2020**, *59*, 15543-15548.

34- “Work-hardening Photopolymer from Renewable Photoactive 3, 3’-(2, 5-Furandiyl) bisacrylic Acid”

Lie, T.; Pellis, A.; Funes-Ardoiz, I.; Sampedro, D.; Macquarrie, D. J.; Farmer, T. J. *ChemSusChem*. **2020**, *13*, 4140.

35- “Established and emerging computational tools to study homogeneous catalysis—From quantum mechanics to machine learning”

Funes-Ardoiz, I.; Schoenebeck, F. *Chem*. **2020**, *6*, 1904-1913.

36- “Photocontrolled Cobalt Catalysis for Selective Hydroboration of α , β -Unsaturated Ketones”

Beltran, F.; Bergamaschi, E.; Funes-Ardoiz, I.; Teskey, C. J. *Angew. Chem. Int. Ed.* **2020**, *59*, 21176-21182.

37- “Consecutive Ligand-Based Electron Transfer in New Molecular Copper-Based Water Oxidation Catalysts”

Gil-Sepulcre, M.; Barrido-Barros, P.; Oldengott, J.; Funes-Ardoiz, I.; Bofill, R.; Benet-Buchholz, J.; Llobet, A. *Angew. Chem. Int. Ed.* **2021**, *60*, 18639-18644.

37- “Consecutive Ligand-Based Electron Transfer in New Molecular Copper-Based Water Oxidation Catalysts”

Gil-Sepulcre, M.; Barrido-Barros, P.; Oldengott, J.; Funes-Ardoiz, I.; Bofill, R.; Benet-Buchholz, J.; Llobet, A. *Angew. Chem. Int. Ed.* **2021**, *60*, 18639-18644.

38- “Dual Photoredox/Cobaloxime Catalysis for Cross-Dehydrogenative α -Heteroarylation of Amines”

Bergamaschi, E.; Weike, C.; Mayerhofer, V. J.; Funes-Ardoiz, I. (corresponding author); Teskey, C. J. *Org. Lett.* **2021**, *23*, 5378-5382.

39- “Hydroalkylation of Unactivated Olefins via Visible-Light-Driven Dual Hydrogen Atom Transfer Catalysis”

Lei, G.; Xu, M.; Chang, R.; Funes-Ardoiz, I. (corresponding author); Ye, J. *J. Am. Chem. Soc.* **2021**, *143*, 11251-11261.

CAPÍTULOS DE LIBRO

1- **Título del capítulo:** “Water as an Oxygen Source for Oxidation Reactions” en el libro “Science of Synthesis: Catalytic Oxidation in Organic Synthesis” (Ed. Prof. Kilian Muñiz, Editorial: Georg Thieme Verlag KG, 2017).

Autores: Garrido-Barros, P.; Funes-Ardoiz, I.; Farràs, P.; Gimbert-Suriñach, C.; Maseras, F.; Llobet, A.

2- **Título del capítulo:** “Introduction to the Mechanistic Scenario in Water Oxidation Catalysis by Transition Metal Complexes” (Ed. James C. Taylor, Editorial: Nova Science Publishers Inc., New York, 2020). ISBN: 978-1-53618-734-2

Autores: Garrido-Barros, P.; Funes-Ardoiz, I. (Corresponding author)

PATENTES

1-**Título:** “Compuestos fotoprotectores análogos de MMA, procedimiento de síntesis y composición que comprende los mismos”. Inventores: Diego Sampedro, Raúl Losantos, Ignacio Funes.

Código de patente: ES-2550374

2-**Título:** “Analogues of mycosporine-like amino acid and use thereof as sunscreens”. Applicant: BASF SE. Inventors: Diego Sampedro, Raúl Losantos, Ignacio Funes-Ardoiz, Thomas Ehlis, Jochen Giesinger, Julie Grume-Lard.

Código de patente: WO 2021/148426 A1

SOFTWARE DESARROLLADO

1- **GoodVibes:** Programa en Python para calcular parámetros termodinámicos a partir de cálculos de estructura electrónica incluyendo correcciones cuasiarmónicas.

Desarrollado por: Paton, R.S.; Funes-Ardoiz, I.; Luchini, G.; Alegre-Requena, J.V.; Guan, Y.; Rodriguez-Guerra, J.

Citas: 43. DOI: 10.5281/zenodo.3346166.

Disponible gratis en: <https://github.com/bobbypaton/GoodVibes>

2- **GARLEEK**: Programa en Python para realizar cálculos QM/MM(ONIOM) usando Gaussian para QM y Tinker para MM.

Desarrollado por: Rodríguez-Guerra Pedregal, J.; Funes-Ardoiz, I.; Sciortino, G.; Sánchez-Aparicio, J.-E.; Ujaque, G.; Lledós, A.; Maréchal, J.-D.; Maseras, F.

Citas: 2. Cite as: *J. Comp. Chem.* **2019**, *40*, 381-386.

Disponible gratis en: <https://github.com/insilichem/garleek>

2- **EasyMECP**: Programa en Python para calcular puntos de cruce de energía mínima (MECP) con el programa Gaussian.

Desarrollado por: Rodríguez-Guerra Pedregal, J.; Funes-Ardoiz, I.; Maseras, F.

Disponible gratis en: <https://github.com/jaimergp/easymecp>

PRESENTACIONES ORALES EN CONFERENCIAS

1- XII Simposio de Investigadores Jóvenes RSEQ-Sigma Aldrich, Barcelona (JIQ-RSEQ), España. 3 -6 Noviembre, 2015.

“A Mechanistic Approach to the Overpotential Control in Cu-Based Water Oxidation Catalysis”

Funes-Ardoiz, I.

2- IX Trobada de Joves Investigadors del Països Catalans, Perpignan (SCQ-UPVD), Francia. 3 -5 Febrero, 2016.

“El Mecanisme de Formació de l’Enllaç O-O en una Nova Família de Catalitzadors de Coure per a Rumpura d’Aigua/ The Mechanism of the O-O Bond Formation in a New Family of Copper Catalyst for Water Splitting”

Funes-Ardoiz, I.

3- IX International School on Organometallic Chemistry “Marcial Moreno Mañas”, Donostia-San Sebastián (UPV-EHU), España. 6 -8, Julio, 2016.

“A Computational Study on the Role of Copper Diacetate in Oxidative Coupling Reactions”

Funes-Ardoiz, I.

4- 6th EuCheMS Chemistry Congress, Sevilla (FIBES), España. 11-15, Septiembre, 2016.

“The Cooperative Effect of Transition Metal Catalysts in the Oxidative Cross-Couplings. A DFT Mechanistic Study” (another oral communication in the special symposium of the European Young Chemistry Awards (EYCA), as a finalist of the competition)

Funes-Ardoiz, I.

5- XIII Simposio de Investigadores Jóvenes de la Real Sociedad Española de Química, Logroño (Unirioja), España. 8 -11, Noviembre, 2016.

“Is One Metal Enough? The Role of Copper Acetate in Oxidative Coupling”

Funes-Ardoiz, I.

6- V COST-CARISMA 2017 Meeting. Lisboa (Sana Malhoa Hotel), Portugal. 6 -8 Marzo, 2017.

“The Single Electron Transfer Mechanism for Oxygen-Oxygen Bond Formation in Copper-Based Water Oxidation Catalysis”.

Funes-Ardoiz, I.; Garrido-Barros, P.; Llobet, A.; Maseras, F.

7- BIST PhD ICIQ Meeting. Tarragona (ICIQ), España. 19 Abril, 2017.

“Computational Chemistry at ICIQ”. (Conferenciante invitado)

Funes-Ardoiz, I.

8- XXXVI Reunión BIENAL de la RSEQ. Sitges (Hotel Melia), España. 25-29 Junio, 2017.

“Single Electron Transfer-Water Nucleophilic Attack Mechanism in Water Oxidation reaction”.

Funes-Ardoiz, I., Garrido-Barros, P.; Llobet, A.; Maseras, F.

9- XXXVI Reunión BIENAL de la RSEQ. Sitges (Hotel Melia), España. 25-29 Junio, 2017.

“Divulgar Durante el Doctorado, ¿Misión Imposible?”

Funes-Ardoiz, I., Garrido-Barros, P.; Maseras, F.

10- International Conference of Computational Methods in Sciences and Engineering 2018 (ICCMSE 2018), The MET Hotel, Thessaloniki, Grecia. 14-18 Marzo, 2018.

“Computational Characterization on the Active Role of the Oxidant in Oxidative Coupling Reactions”. (Conferenciante invitado)

Funes-Ardoiz, I.

11- Girona Seminar: Predictive Catalysis, Transition-Metal Reactivity by Design, Girona, España. 3-6 Abril, 2018.

“Understanding the Active Role of the Oxidant in the Oxidative Coupling of Benzoic Acid and Alkyne”.

Funes-Ardoiz, I.

12- European Colloquium on Inorganic Reaction Mechanisms 2018, Barcelona, España. 8-11 Julio, 2018.

“Exploring the Mechanism of Ru-Cu Cooperative Catalysis in the Oxidative Homocoupling of Carbazoles”.

Funes-Ardoiz, I.

13- Gordon Research Seminar on Green Chemistry 2018, Rey Don Jaime Grand Hotel en Castelldefels, España. 28-29 Julio, 2018; Gordon Research Conference on Green Chemistry 2018, Rey Don Jaime Grand Hotel in Castelldefels, España. 29 Julio-3 Agosto, 2018.

Charla (GRS) y póster (GRC): “Computational Insight into the Single Electron Transfer-Water Nucleophilic Attack Mechanism in Copper based Water Oxidation Catalysis”.

Funes-Ardoiz, I.

PREMIOS

- 1- Premio “Catalysis Science and Technology” a la mejor presentación oral en el Girona Seminar 2018.
- 2- Premio 2017 Josep Castells Award a la mejor tesis doctoral en Cataluña de la Real Sociedad Española de Química.
- 3- Primer premio y premio especial del público en el concurso de divulgación científica: “Vols saber què investigo? (2015)” con el monólogo “Rompamos el agua (splitting the water)” organizado por la Universitat Rovira i Virgili. Video disponible en:
https://www.youtube.com/watch?v=S61Gzxx0W08&list=PL8yyYJSAXdwluigrH_bTNw9AXGJi0jao
- 4- Ganador del concurso científico “Somos científicos, sácanos de aquí” (Edición española), Noviembre 2016.
- 5- 2º Premio en el concurso de innovación Falling Walls Lab Barcelona 2017. 12 septiembre de 2017.
- 6- Medalla de plata en la olimpiada española de química, 2009.

BECAS Y AYUDAS COMPETITIVAS

- 1- Beca “Iniciación a la Investigación (Introduction to research)” bajo la supervisión del Dr. Diego Sampedro en la Universidad La Rioja. De 1/12/2011 a 30/06/2012.
- 2- Beca ICIQ Summer Fellowship bajo la supervision del Prof. Feliu Maseras. Instituto Catalán de Investigación Química. Verano 2012 (3 meses).
- 3- Ayuda para estudios de máster (“Ayuda de estudio del Institut Català d’Invetigació Química”) bajo la supervision del Prof. Feliu Maseras. Instituto Catalán de Investigación Química. 2013-2014

4- Ayuda predoctoral para centros/unidades de excelencia Severo Ochoa (2014) y de Periodo de Orientación Postdoctoral. Referencia: SVP-2014-068662). 2014-2018

5- Beca postdoctoral Humboldt de la Fundación Alexander Von Humboldt (24 meses) en la universidad RWTH Aachen (Alemania).

HABILITACIÓN ACADÉMICA

1- Acreditación de la Agencia Nacional de Evaluación de la Calidad y Acreditación (ANECA) como “Profesor Ayudante Doctor”. Mayo, 2018.

2- Acreditación de la Agencia Nacional de Evaluación de la Calidad y Acreditación (ANECA) como “Profesor Contratado Doctor”. Diciembre, 2018.

EXPERIENCIA DOCENTE

1- Profesor asistente en la asignatura de máster “Angewandte Computer Chemie (Química Computacional Aplicada)” 3 créditos ECTS credits. Universidad RWTH Aachen University. 2019-2020.

2- Supervisión de proyectos de máster en la Universidad RWTH Aachen:

Nombre del estudiante: Julian Hüffel

Número de matrícula: 380507

Fechas: del 13.03.2019 al 10.05.2019

Título del proyecto: “Computational characterization of cross-coupling organic reactions”.

Duración: 30 días + 2 semanas extra

Presentación de resultados: 03.06.2019

Nombre del estudiante: Clara Nussbaumer

Número de matrícula: 344098

Fechas: del 06.05.19 al 28.06.19

Título del proyecto: Computational study of copper-catalyzed C-C bond cleavage.

Duración: 2 meses

Presentación de resultados: 12.07.19

Nombre del estudiante: Hendrik Simon

Número de matrícula: estudiante visitante de la Technische Universität Berlin.

Fechas: del 07.10.19 al 07.12.19

Título del proyecto: Computational study of homogeneous Pd nanocluster catalysis of Heck reaction.

Duración: 2 meses

Presentación de resultados: 07.12.19

Nombre del estudiante: Sander Folkerts

Número de matrícula: 355785

Fechas: del 14.11.19 al 23.01.2020

Título del proyecto: Computational study of homogeneous Pd nanocluster catalysis of Heck reaction.

Duración: 2 meses

Presentación de resultados: 23.01.2020

3- Supervisión de tesis de máster en la Universidad RWTH Aachen (en progreso):

Nombre del estudiante: Julian Hüffel

Número de matrícula: 380507

Fechas: del 21.10.2019 al 21.04.2020

Título del proyecto: Applied Machine Learning in Computational Chemistry

Duración: 6 meses

Presentación de resultados: 21.04.2020

ACTIVIDADES DE DIVULGACIÓN

1- **Participación en el concurso de monólogos científicos “Vols saber què investigo? (2015)”** con el monólogo “Rompamos el agua”. Noviembre, 2015. Organizado por la Unidad de Comunicación de la Ciencia de la universidad Rovira i Virgili.

2- **Monólogos científicos en el instituto Martí i Franquès.** 22 de abril, 2016. Organizado por la Unidad de Comunicación de la Ciencia de la universidad Rovira i Virgili.

3- **Participación en la Fiesta de la Ciencia Barcelona 2016-charla “Trenquem l'aigua” y el taller “Catàlisi Exprès”** 18-19 de junio, 2016. Organizado por Barcelona Ciencia and Ayuntamiento de Barcelona en el parque de la Ciutadella.

4- **Participación en el concurso de monólogos científicos “Vols saber què investigo? como jurado”** y con el monólogo “Fotoprotégete”. Noviembre, 2016. Organizado por la Unidad de Comunicación de la Ciencia de la universidad Rovira i Virgili. Vídeo disponible en (a partir de 1 hora y 21 minutos): <https://www.youtube.com/watch?v=e6LyjRjkOp4&t=4086s>

5- **Participación en la actividad “Dia de la Ciencia a les Escoles” en el INS Martí l'Humà en Montblanc con la charla “¿Se puede ser químico sin bata de laboratorio?”** 16 de noviembre, 2016. Organizado por la “Fundació Catalana per a la Recerca i la Innovació”.

6- **Participación en el concurso de divulgación científica “Somos científicos sácanos de aquí” (edición española).** Noviembre, 2016. Zona “Medio Ambiente”.

7- **Charla titulada “Mi experiencia investigadora” en el IES Benjamín de Tudela in Tudela** 7 de diciembre, 2016. Organizado por IES Benjamín de Tudela.

8- **Participación en la “Fira Tastet de Ciència 2017” con el monólogo titulado “Fotoprotégete” en el Centro de Lectura de Reus.** 17 de mayo, 2017. Organizado por el Centre de Recursos pedagògics Baix Camp.

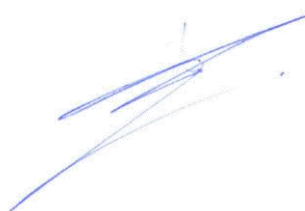
9- **Participación en el simposio “Seguim Bojos per la Química” con la charla “Se puede ser químico sin bata de laboratorio?”**, 7 de Julio, 2017. ICIQ, Tarragona.

10- **Participación en el concurso “Falling Walls Lab Barcelona” con la charla “Breaking the Wall of Energy Production”**, 12 de septiembre, 2017. UPF, Barcelona.

11- **Participación en la actividad “Dia de la Ciencia a les Escoles” en el INS Joan Puig i Ferrater en La Selva del Camp con la charla “¿Se puede ser químico sin bata de laboratorio?”** 15 de noviembre, 2017. Organizado por la “Fundació Catalana per a la Recerca i la Innovació”..

12- **Participación en el festival Pint of Science 2018 (edición Tarragona) en la Vinatería Clot Martell con la charla “Imitemos a las plantas”**. 14 de mayo, 2018. Organizado por Pint of Science España.

Firma:

A handwritten signature in blue ink, consisting of several overlapping, fluid strokes that form a cursive-like shape.

Dr. Ignacio Funes Ardoiz
Aachen, 04/03/2020