

CURRICULUM VITAE – JULEN MUNÁRRIZ

PERSONAL INFORMATION

NAME: **JULEN MUNÁRRIZ**

BIRTH DATE: 3rd April 1992

NACIONALITY: Spanish

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MAILING ADDRESS: Department of Chemistry and Biochemistry, UCLA



CURRENT POSITION

Postdoctoral researcher at the University of California, Los Angeles, Department of Chemistry and Biochemistry. Advisor: Prof. Anastassia Alexandrova (ana@chem.ucla.edu)

EDUCATION

2015 – 2019 **PhD** in Physical Chemistry, Universidad de Zaragoza (Spain). “Computational Catalysis of Homogeneous and Heterogeneous Systems: New Insights into the activation of Small Molecules”. Advisor: Dr. Victor Polo. International doctorate, Excellent Cum laude.

2014 – 2016 **Master’s Degree:** European Master in Theoretical Chemistry and Computational Modelling. University of Valencia, Spain (three months stay in KU Leuven, Belgium).

- *Master’s Dissertation:* “A mechanistic study of the alpha-hydrosilylation of terminal alkynes catalyzed by Rh complexes”. Advisor: Dr. Victor Polo and Prof. Dr. Jeremy Harvey (jeremy.harvey@chem.kuleuven.be).
- *Average score:* 9.38/10.

2010 – 2014 **Bachelor’s Degree** in Chemistry. Universidad de Zaragoza.

- *Bachelor’s dissertation:* “Computational study of the mechanism, regioselectivity and stereochemistry of the hydrosilylation of terminal alkynes catalyzed by organometallic complexes”. Advisor: Dr. Victor Polo.
- *Average score:* 9.40/10.

FELLOWSHIPS

- 2015 – 2019** Programa de Formación de Profesorado Universitario. Spanish Ministry of Education Fellowship.
- 2015** JAE INTRO 2015 (Introduction to Research Grant for Graduate Students). Spanish Research Council (“Consejo Superior de Investigaciones Científicas, CSIC”). Project: “Design of Novel Catalysts for Sustainable Chemical Processes”. Advisor: Prof. Dr. Jesús Pérez Torrente (perez@unizar.es), 10/01/2015 – 10/25/2015.
- 2014** Beca de Introducción a la Investigación (Introduction to Research Fellow for University Students). Instituto de Nanociencia de Aragón (INA), Universidad de Zaragoza. Project: “Theoretical Chemistry as a tool for understanding biochemical systems”. Advisor: Prof. Dr. Javier Galbán (jgalban@unizar.es), 07/09/2014 – 09/12/2014.
- 2013 – 2014** Beca de Colaboración en Departamentos Universitarios (*Assistantship in the Physical Chemistry Department of the University of Zaragoza*). Spanish Ministry of Education, 09/01/2013 – 05/31/2014.

AWARDS

- 2017** Research stay in Sorbonne University, France. Spanish Ministry of Education and CAI – Ibercaja Foundation.
- 2016** Research stay in Sorbonne University, France. Spanish Ministry of Education.
- 2015** Research stay in KU Leuven, Belgium. CAI – Ibercaja Foundation.
- 2014** Premio Extraordinario de Fin de Grado (Extraordinary Award conferred to the best student of the Degree in Chemistry). Faculty of Science, Universidad de Zaragoza.

RESEARCH STAYS

- 2018** Laboratoire de Chimie Théorique, Sorbonne Université, Paris, France. Advisor: Dr. Julia Contreras-García (contrera@lctjussieu.fr). 08/04/2018 – 07/09/2018 (three months).
- 2017** Laboratoire de Chimie Théorique, Sorbonne Université, Paris, France. Advisor: Dr. Julia Contreras-García. 05/01/2017 – 07/31/2017 (three months).
- 2016** Chemistry Department, KU Leuven, Leuven, Belgium. Advisor: Prof. Dr. Jeremy Harvey. 15/03/2016 – 15/06/2016 (three months).

PARTICIPATION IN FUNDED RESEARCH PROJECTS

- “Activación de NH_3 y CO_2 por complejos de rodio e iridio y su aplicación en el desarrollo de procesos catalíticos para la síntesis de compuestos de alto valor añadido.” 01/01/2016 – 12/31/2018. Financed by the Spanish Ministry of Economy, Industry and Competivity (MINECO), 112651 €. PI: Victor Polo and Miguel Ángel Casado.
- “Grupo de Referencia Catálisis Homogénea por Compuestos Organometálicos” 01/01/2017 – 12/31/2019. Financed by the Aragon Government, 38529 €. PI: Jesús Julián Pérez Torrente.

PUBLICATIONS

- 17. Julen Munárriz,*** Rubén Laplaza, Ángel M. Pendás, Julia Contreras-García.*
A first step towards quantum energy potentials of electron pairs
Phys. Chem. Chem. Phys. 2019, 21, 4215–4223
- 16. Julen Munárriz,** Rubén Laplaza, Victor Polo.*
A bonding evolution theory study on the catalytic Noyori hydrogenation reaction
Mol. Phys. 2018, DOI: 10.1080/00268976.2018.1542168. Invited paper in the honour of Prof. Dieter Cremer.
- 15. Amaia Iturmendi,** Manuel Iglesias,* **Julen Munárriz,** Victor Polo, Vincenzo Passarelli, Jesús J. Pérez-Torrente, Luis A. Oro.*
Highly Efficient Ir-Catalyst for the Solventless Dehydrogenation of Formic Acid: The Key Role of an N-heterocyclic Olefin
Green Chem. 2018, 20, 4875–4879.
- 14. Julen Munárriz,*** Federico A. Rabuffetti, Julia Contreras-García.*
Building Fluorinated Hybrid Crystals: Understanding the role of Noncovalent Interactions
Cryst. Growth Des. 2018, 18, 6901–6910.
- 13. Julen Munárriz,*** Victor Polo, Jose Gracia.*
On the Role of Ferromagnetic Interactions in Highly Active Mo-based Catalysts for Ammonia Synthesis
ChemPhysChem 2018, 19, 2843–2847.
- 12. Jose Gracia,*** Ryan Sharpe, **Julen Munárriz.**
Principles determining the activity of magnetic oxides for electron transfer reactions
J. Catal. 2018, 361, 331–338.
- 11. Ryan Sharpe,*** **Julen Munárriz,** Tingbin Lim, Yunzhe Jiao, J. W. (Hans) Niemantsverdriet, Victor Polo, Jose Gracia.*
Orbital Physics of Perovskites for the Oxygen Evolution Reaction
Top. Catal. 2018, 61, 267–275.

10. **Julen Munárriz**, Ederley Velez, Miguel Ángel Casado, Victor Polo.*
Understanding the reaction mechanism of the oxidative addition of ammonia by (PXP)Ir(i) complexes: The role of the X group
Phys. Chem. Chem. Phys. 2018, 20, 1105–1113.
9. Jose Gracia,* **Julen Munárriz**, Victor Polo, Ryan Sharpe, Yunzhe Jiao, J. W. (Hans) Niemantsverdriet, Tingbin Lim.
Analysis of the Magnetic Entropy in Oxygen Reduction Reactions Catalysed by Manganite Perovskites
ChemCatChem 2017, 9, 3358–3363.
8. Lucía González, Rosa María Tejedor, Eva Royo, Blanca Gaspar, **Julen Munárriz**, Anjana Chanthapally, José Luis Serrano, Jagadeesha J. Vittal, Santiago Uriel.*
Two-Dimensional Arrangements of Bis(haloethynyl)benzenes Combining Halogen and Hydrogen Interactions
Cryst. Growth Des. 2017, 17, 6212–6223.
7. Laura Rubio-Pérez, Manuel Iglesias,* **Julen Munárriz**, Victor Polo, Vincenzo Passarelli, Jesús J. Pérez-Torrente, Luis A. Oro.*
A well-defined NHC–Ir(III) catalyst for the silylation of aromatic C–H bonds: substrate survey and mechanistic insights
Chem. Sci. 2017, 8, 4811–4822.
6. Amaia Iturmendi, Manuel Iglesias,* **Julen Munárriz**, Victor Polo, Jesús J. Pérez-Torrente, Luis A. Oro.*
Efficient preparation of carbamates by Rh-catalysed oxidative carbonylation: unveiling the role of the oxidant
Chem. Commun. 2017, 53, 404–407.
5. Amaia Iturmendi, Nestor García, E. A. Jaseer, **Julen Munárriz**, Pablo J. Sanz Miguel, Victor Polo, Manuel Iglesias,* Luis A. Oro.*
N-Heterocyclic olefins as ancillary ligands in catalysis: a study of their behaviour in transfer hydrogenation reactions
Dalton Trans. 2016, 45, 12835–12845.
4. Laura Rubio-Pérez, Manuel Iglesias,* **Julen Munárriz**, Victor Polo, Jesús J. Pérez-Torrente, Luis A. Oro.*
Efficient Rhodium-Catalyzed Multicomponent Reaction for the Synthesis of Novel Propargylamines
Chem. Eur. J. 2015, 21, 17701–17707.
3. Nestor García, E. A. Jaseer, **Julen Munárriz**, Pablo J. Sanz Miguel, Victor Polo, Manuel Iglesias,* Luis A. Oro.*
An Insight into Transfer Hydrogenation Reactions Catalysed by Iridium(III) Bis-N-heterocyclic Carbenes

- Eur. J. Inorg. Chem.* 2015, 4388–4395.
2. Laura Rubio-Pérez, Manuel Iglesias,* **Julen Munárriz**, Victor Polo, Pablo J. Sanz Miguel, Jesús J. Pérez-Torrente, Luis A. Oro.*
A bimetallic iridium(II) catalyst: $\{[Ir(IDipp)(H)]_2\}[BF_4]_2$ (IDipp = 1,3-bis(2,6-diisopropylphenylimidazol-2-ylidene))
Chem. Commun. 2015, 51, 9860–9863.
 1. Guillermo Lázaro, Francisco J. Fernández-Alvarez,* **Julen Munárriz**, Víctor Polo, Manuel Iglesias, Jesús J. Pérez-Torrente, Luis A. Oro.*
Orthometallation of N-substituents at the NHC ligand of $[R(Cl)(COD)(NHC)]$ complexes: its role in the catalytic hydrosilylation of ketones
Catal. Sci. Technol. 2015, 5, 1878–1887.

CONFERENCE PRESENTATIONS

13. IX National Conference BIFI 2019, Zaragoza, Spain (2018).
Oral presentation, “*The Role of Magnetic Interactions in Perovskite-Catalysed Electron Transfer Reactions*”.
12. 8ª Jornada de Jóvenes Investigadores (Química y Física) de Aragón, Zaragoza, Spain (2018).
Poster, “*Magnetic Interactions Meet Catalyst Design*”.
11. Second European Symposium on Chemical Bonding (ESCB2), Oviedo, Spain (2018).
Oral presentation, “*Valence shell electron pair repulsion theory extended to core electrons*”.
10. 6th Workshop on Theoretical Chemistry and Computational Modelling, Toledo, Spain (2018).
Oral presentation, “*Noncovalent Interactions as a tool for understanding Structure of Bimetallic Fluorinated Hybrid Crystals*”.
9. 11th Congress on Electronic Structure: Principles and Applications (ESPA 2018), Toledo, Spain (2018).
Poster, “*Topology as a tool for constructing energy models*”.
8. 16th International Congress on Quantum Chemistry, Menton, France (2018).
Poster, “*Energy Models from Valence Shell Electron Pair Repulsion*”.
7. 11th European Conference on Theoretical Chemistry and Computational Modelling, Barcelona, Spain (2017).
Poster, “*Tuning electronic factors controlling oxidative addition of ammonia N-H bond to Ir(I) PXP pincer complexes*”.

6. 11th Triennial Congress on the World Association of Theoretical and Computational Chemists, Munich, Germany (2017).
Poster, “Computationally guided design of transition metal PXP pincer complexes for NH₃ fixation”.
5. 7^a Jornada de Jóvenes Investigadores (Química y Física) de Aragón, Zaragoza, Spain (2016).
Oral presentation, “Estudio mecanístico de nuevos catalizadores de Ir(III)-NHC para sililación selectiva de enlaces C-H”.
4. XXXIV Congress of the Organometallic Chemistry Specialized Group of the Real Sociedad Española de Química, Girona, Spain (2016).
Poster, “Influence of N-Heterocyclic Olefins in Catalytic Hydrogen Transfer Reactions. A DFT Theoretical Study”.
3. 10th Congress on Electronic Structure: Principles and Applications (ESPA 2016), Castellón, Spain (2016).
Poster, “A mechanistic study of the α -hydrosilylation of terminal alkynes catalysed by bis-NHC carbene Rh(III) catalysts”.
2. 5th Workshop on Theoretical Chemistry and Computational Modelling, Castellón, Spain (2016).
Oral presentation, “Understanding the selectivity of α -hydrosilylation of terminal alkynes catalyzed by bis-NHC carbene Rh, Ir complexes: A DFT theoretical study”.
1. 9th Congress on Electronic Structure: Principles and Applications 2016 (ESPA 2014), Badajoz, Spain (2014).
Poster, “A mechanistic Study on the hydrosilylation of phenylacetylene catalysed by Ir complex”.

TEACHING AND MENTORING EXPERIENCE

- 180 hours of University teaching, including General Chemistry, Physical Chemistry and Computational Chemistry.
- Mentoring experience:
 - Summer Internship in Computational Chemistry. Student: Maria Pilar Ibáñez Millan (undergraduate), 06/28/2018 – 07/27/2018 (100 hours).
- Scientific dissemination:
 - Immersion Weeks for Secondary School Students at the Faculty of Science of the Universidad de Zaragoza. Academic years 2013–2014 and 2015–2016.
 - Science Week at *Colegio de España, Cité Universitaire*, Paris, France. Academic years 2016–2017 and 2017–2018.

LANGUAGES SKILLS

- **Spanish:** Native tongue.
- **English:** Level C1 (*Certificate in Advanced English, Cambridge University CAE*).
- **French:** Level B2 (DELF-B2 certificate).