JAVIER HERAS DOMINGO

Ph.D. in Chemistry

07-February-1991
Citizenship: Barcelona (Spain)
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EXPERIENCE

Lecturer (Assistant Professor)
University of Barcelona - Department of Inorganic Chemistry
June 2025 - Currently | Barcelona, Spain

Adjunct Professor
Autonomous University of Barcelona - Chemistry Department
October 2024 - June 2025 | Bellaterra Campus, Barcelona (Spain)

Postdoctoral Researcher
Prof. Núria López - Institute of Chemical Research of Catalonia (ICIQ)
January 2023 - June 2025 | Tarragona, Spain

Postdoctoral Researcher
Prof. Zachary Ulissi Group - Carnegie Mellon University
February 2020 - November 2022 | Pittsburgh, Pennsylvania, (USA)

EDUCATION

Ph.D. Degree In Theoretical Chemistry (International Mention)
Prof. Mariona Sodupe and Prof. Xavier Solans-Monfort Autonomous University of Barcelona
January 2016 - January 2020 | Bellaterra Campus, Barcelona (Spain)

Master Degree of Industrial Chemistry and Introduction to Chemical Research
Autonomous University of Barcelona
2014 - September 2015 | Bellaterra Campus, Barcelona (Spain)

Bachelor Degree in Chemistry (Mention in Materials Science)
Autonomous University of Barcelona
2009 - June 2014 | Bellaterra Campus, Barcelona (Spain)

DISTINCTIONS

- Associate Professor Accreditation - **AQU (2025)**

SKILLS

- **Density Functional Theory Codes:** VASP, CP2K, Gaussian and ORCA
- **Programming Languages:** Python, HPC-SLURM and Bash
- **Software Development:** Conda, Git, Docker, MongoDB and Kubernetes
- **Frameworks and Libraries:** Atomate, FireWorks, Custodian, Pymatgen, ASE, PyMongo, and PyTorch
- **Languages:** Spanish, Catalan, English and German

OPEN SOURCED PROJECTS

WhereWulff: A semi-autonomous workflow for systematic catalyst surface reactivity under reaction conditions

https://github.com/ulissigroup/wherewulff

>_ Automated and scalable Workflow for materials high-throughput computational screening with applications in multi-metallic oxides discovery for the oxygen evolution reaction (OER).

FireWorks and Atomate Tutorial

https://github.com/jherasdo/FireWorks-Atomate-Tutorial

>_ Workshop on FireWorks and Atomate libraries for materials modeling and catalysis at Prof. Zachary Ulissi's research group.

Pythonic Chemistry

https://github.com/jherasdo/pythonic-chemistry

>_ Python programming language course for chemistry students at the PhD level. Developed under the ICIQ-SHARP Program.

VibraCLIP

https://github.com/jherasdo/vibraclip

>_ A tool for Smart Multi-modal Characterization of molecules, leveraging contrastive learning to align structural (graph) and vibrational (IR, Raman) information.

RESEARCH CONTRIBUTIONS

Publications

- Rocabert-Oriols, P., N. López, and **J. Heras-Domingo** (**2025**). "Multi-Modal Contrastive Learning for Chemical Structure Elucidation with VibraCLIP". in: *ChemRxiv*.
- **J. Heras-Domingo** and D. Garay-Ruiz (**2024**). "Pythonic Chemistry: The Beginner's Guide to Digital Chemistry". In: *Journal of Chemical Education*.
- Abed, J., **J. Heras-Domingo**, R. Y. Sanspeur, M. Luo, W. Alnoush, D. M. Meira, H. Wang, J. Wang, J. Zhou, D. Zhou, et al. (**2024**). "Pourbaix Machine Learning Framework Identifies Acidic Water Oxidation Catalysts Exhibiting Suppressed Ruthenium Dissolution". In: *Journal of the American Chemical Society*.
- Rossi, K., A. Ruiz-Ferrando, D. F. Akl, V. G. Abalos, **J. Heras-Domingo**, R. Graux, X. Hai, J. Lu, D. Garcia-Gasulla, N. López, et al. (**2024**). "Quantitative Description of Metal Center Organization and Interactions in Single-Atom Catalysts". In: *Advanced Materials* 36.5, p. 2307991.
- Garrison, A. G., **J. Heras-Domingo**, J. R. Kitchin, G. dos Passos Gomes, Z. W. Ulissi, and S. M. Blau (**2023**). "Applying Large Graph Neural Networks to Predict Transition Metal Complex Energies Using the tmQM_wB97MV Data Set". In: *Journal of Chemical Information and Modeling* 63.24, pp. 7642–7654.
- Romero, N., D. Fenoll, L. Gil, S. Campos, J. Creus, G. Martí, **J. Heras-Domingo**, V. Collière, C. A. Mesa, S. Gimenez, et al. (**2023**). "Ru-based nanoparticles supported in carbon nanotubes for electrocatalytic hydrogen evolution: structural and electronic effects". In: *Inorganic Chemistry Frontiers*.
- Sanspeur, R. Y., **J. Heras-Domingo**, J. R. Kitchin, and Z. Ulissi (**2023**). "WhereWulff: A Semiautonomous Workflow for Systematic Catalyst Surface Reactivity under Reaction Conditions". In: *Journal of Chemical Information and Modeling* 63.8, pp. 2427–2437.
- Tran, R., J. Lan, M. Shuaibi, B. M. Wood, S. Goyal, A. Das, **J. Heras-Domingo**, A. Kolluru, A. Rizvi, N. Shoghi, et al. (**2023**). "The Open Catalyst 2022 (OC22) dataset and challenges for oxide electrocatalysts". In: *ACS Catalysis* 13.5, pp. 3066–3084.
- Chanussot, L., A. Das, S. Goyal, T. Lavril, M. Shuaibi, M. Riviere, K. Tran, **J. Heras-Domingo**, C. Ho, W. Hu, A. Palizhati, A. Sriram, B. Wood, J. Yoon, D. Parikh, C. Zitnick, and Z. Ulissi (**2021**). "Erratum: The Open Catalyst 2020 (OC20) Dataset and Community Challenges". In: *ACS Catalysis* 11 (21).
- Chanussot, L., A. Das, S. Goyal, T. Lavril, M. Shuaibi, M. Riviere, K. Tran, **J. Heras-Domingo**, C. Ho, W. Hu, A. Palizhati, A. Sriram, B. Wood, J. Yoon, D. Parikh, C. Zitnick, and Z. Ulissi (**2021**). "Open Catalyst 2020 (OC20) Dataset and Community Challenges". In: *ACS Catalysis* 11 (10).
- González, D., **J. Heras-Domingo**, M. Sodupe, L. Rodríguez-Santiago, and X. Solans-Monfort (**2021**). "Importance of the oxyl character on the IrO2 surface dependent catalytic activity for the oxygen evolution reaction". In: *Journal of Catalysis* 396.
- González, D., B. Camino, **J. Heras-Domingo**, A. Rimola, L. Rodríguez-Santiago, X. Solans-Monfort, and M. Sodupe (**2020**). "BCN-M: A Free Computational Tool for Generating Wulff-like Nanoparticle Models with Controlled Stoichiometry". In: *Journal of Physical Chemistry C* 124 (1).

- Lebedev, D., R. Ezhov, **J. Heras-Domingo**, A. Comas-Vives, N. Kaeffer, M. Willinger, X. Solans-Monfort, X. Huang, Y. Pushkar, and C. Copéret (**2020**). "Atomically Dispersed Iridium on Indium Tin Oxide Efficiently Catalyzes Water Oxidation". In: *ACS Central Science* 6 (7).
- Zitnick, C. L., L. Chanussot, A. Das, S. Goyal, **J. Heras-Domingo**, C. Ho, W. Hu, T. Lavril, A. Palizhati, M. Rivière, M. Shuaibi, A. Sriram, K. Tran, B. Wood, J. Yoon, D. Parikh, and Z. Ulissi (**2020**). "An Introduction to Electrocatalyst Design using Machine Learning for Renewable Energy Storage". In: *ArXiv* abs/2010.09435.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2019**). "Interaction between Ruthenium Oxide Surfaces and Water Molecules. Effect of Surface Morphology and Water Coverage". In: *Journal of Physical Chemistry C* 123 (13).
- González, D., **J. Heras-Domingo**, S. Pantaleone, A. Rimola, L. Rodríguez-Santiago, X. Solans-Monfort, and M. Sodupe (**2019**). "Water Adsorption on MO2 (M= Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects". In: *ACS Omega* 4 (2).
- Luis-Barrerra, J., R. Cano, G. Imani-Shakibaei, **J. Heras-Domingo**, J. Perez-Carvajal, I. Imaz, D. Maspoch, X. Solans-Monfort, J. Aleman, and R. Mas-Balleste (**2019**). "Switching acidic and basic catalysis through supramolecular functionalization in a porous 3D covalent imine-based material". In: *Catalysis Science and Technology* 9 (21).

Conferences Participation

- **Heras-Domingo, J.**, A. Ruiz-Ferrando, and N. López (**2025**). "Dexifrant el Potencial de L'EXAFS: Aprenentatge Automatic per a Dades Espectroscopiques". In: *2 Reunio de Quimica Teorica I Computacional, RQTC. Oral Communication*. Barcelona.
- **Heras-Domingo, J.**, A. Ruiz-Ferrando, S. Pollit, A. Clark, S. Mitchell, O. Safonova, J. Pérez-Ramírez, and N. López (**2024**). "Smart Characterization of Heterogeneous Catalysts: EXAFS for Single Atom Catalysts". In: *18th ICC: International Congress on Catalysis. Oral Communication*. Lyon, France.
- **Heras-Domingo, J.**, A. Ruiz-Ferrando, S. Pollit, A. Clark, S. Mitchell, O. Safonova, J. Pérez-Ramírez, and N. López (**2024**). "Unlocking the potential of EXAFS: Machine Learning Approaches for Spectroscopic Data". In: *MLM4MS: Machine Learning Modalities for Materials Science. Oral Communication and Poster*. Ljubljana, Slovenia.
- **Heras-Domingo, J.**, A. Ruiz-Ferrando, S. Pollit, A. Clark, S. Mitchell, O. Safonova, J. Pérez-Ramírez, and N. López (**2024**). "Unlocking the potential of EXAFS: Machine Learning Approaches for Spectroscopic Data". In: *RACXS: Recent Advances in Computer-aided X-ray Spectroscopy. Oral Communication.* Helsinki, Finland.
- **Heras-Domingo, J.**, A. Ruiz-Ferrando, S. Pollit, A. Clark, S. Mitchell, O. Safonova, J. Pérez-Ramírez, and N. López (**2024**). "Unlocking the potential of EXAFS: Machine Learning Approaches for Spectroscopic Data". In: *AI4AM: Artificial Intelligence for Advanced Materials. Oral Communication*. Barcelona, Spain.
- **Heras-Domingo, J.** (**2024**). "Scientific Workflows for Theoretical Chemistry and AI". in: *DAEMON COST Action, General Meeting. Oral Communication*. The Hague, Netherlands.
- **Heras-Domingo, J.**, A. Ruiz-Ferrando, and N. Lopez (**2023**). "Automated workflows and ML for structure elucidation of platinum single atom catalysts". In: *XXXIX-RSEQ-Bineal de Química Congress. Oral Communication*. Zaragoza, Spain.
- **Heras-Domingo, J.**, R. Y. Sanspeur, and Z. Ulissi (**2022**). "WhereWulff: An Autonomous Workflow to Democratize and Scale Complex Material Discovery for Electrocatalysis". In: *The 27th North American Catalysis Society Meeting. Oral Communication*. New York, USA.
- Lebedev, D., **J. Heras-Domingo**, A. Comas-Vives, X. Solans-Monfort, and C. Copéret (**2019**). "Single-Site Ir@ITO Catalyst for Water Splitting". In: *XXXVII-RSEQ-Bienal de Química Congress. Poster Presentation*. San Sebastian, Spain.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2018**). "From Surface to Nanoparticles: Ruthenium Oxide Systems and their Interaction with water". In: *Doctoral Workshop of the PhD Program in Chemistry. Flash Presentation + Poster*. Barcelona, Spain.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2018**). "From Surface to Nanoparticles: Ruthenium Oxide Systems and their Interaction with water". In: *International Congress of Quantum Chemistry (ICQTC) Congress. Poster Presentation*. Menton, France.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2017**). "Study of the interactions between ruthenium oxide surfaces and water molecules". In: *XXXVI-RSEQ-Bienal de Química Congress. Poster Presentation*. Sitges, Spain.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2017**). "Study of the interactions between ruthenium oxide surfaces and water molecules". In: *World Association of Theoretical and computational Chemists (WATOC) Congress. Poster Presentation*. München, Germany.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2016**). "Study of the interactions between ruthenium oxide surfaces and water molecules". In: *Xarxa de Quimica Teorica I Computational. Oral Communication*. Barcelona.
- **Heras-Domingo, J.**, M. Sodupe, and X. Solans-Monfort (**2016**). "Study of the interactions between ruthenium oxide surfaces and water molecules". In: *Electronic Structure Principles and Applications (ESPA). Poster Presentation*. Castellón de la Plana, Spain.

Workshops

- *Fireworks/Atomate Tutorial* (**2022**). Contrib. Oral Communication. Online: Prof. Z. Ulissi's research group (CMU).
- *Deep Learning for Surface Science* (**2021**). Contrib. Oral Communication. Online: Physical Chemistry Department (UAB).
- *Machine learning: How to coarse-grain* (**2020**). Contrib. Assistance. Online: CECAM-DE-SMSM.
- *Machine Learning for Material Science* (**2019**). Contrib. Assistance. Helsinki, Finland: Aalto University.
- *Introduction to Statistical Computing in Python* (**2017**). Contrib. Assistance. Barcelona, Spain: Servei de Genòmica I Bioinformàtica.
- *Vienna Ab Initio Simulation Package (VASP)* (**2016**). Contrib. Assistance. Rennes, France: ICAMM Workshop.

TEACHING AND MENTORING

Teaching (2023-2024) ICIQ SHARP Program for PhD students
Total Hours of Teaching: 20
Area: Digital Chemistry
Subjects:
- ➢ Pythonic Chemistry
- ➢ Artificial Intelligence for Chemistry

Teaching (2024-2025) at the Autonomous University of Barcelona (UAB)
Total Hours of Teaching: 131
Area: Physical Chemistry
Subjects:
- ➢ Physical-Chemistry Laboratories
- ➢ Chemical Bonding and Structure of Matter

Teaching (2015/2019) at Autonomous University of Barcelona (UAB)
Total Hours of Teaching: 469
Area: Physical Chemistry
Subjects:
- ➢ Physical-Chemistry Laboratories
- ➢ Chemical Thermodynamics
- ➢ Spectroscopy
- ➢ Chemical Reactivity
- ➢ Fundamentals of Chemistry