

# JAVIER HERAS DOMINGO

Ph.D. in Theoretical Chemistry

📅 07-February-1991

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🌐 <https://github.com/jherasdo>



## EXPERIENCE

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Postdoctoral Researcher

**Prof. Zachary Ulissi Group - Carnegie Mellon University**

📅 February 2020 - Currently

📍 Pittsburgh, Pennsylvania, (USA)

- High-throughput computational screening of multi-metallic oxides to discover acid- stable OER catalysts
- Machine learning applications to optimize OER catalytic property using computational and experimental data
- Graph neural networks for transition metal complexes

## EDUCATION

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Ph.D. Degree In Theoretical Chemistry (International Mention)

**Autonomous University of Barcelona**

📅 January 2016 - January 2020

📍 Bellaterra Campus, Barcelona (Spain)

- Thesis Title: "Modeling of RuO<sub>2</sub> Surfaces and Nanoparticles: *Their potential use as catalysts for the oxygen evolution reaction.*"
- Supervisors: Prof. Dr. Mariona Sodupe and Dr. Xavier Solans-Monfort
- International Mention: Research internship at Prof. Christophe Copéret Research Group (ETH Hönggerberg, Zürich, Switzerland)
- Qualification: Excellent (*Cum Laude*)

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)

## SKILLS

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- **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, Pymatgen, ASE, PyMongo, and PyTorch
- **Languages:** Spanish, Catalan, English and German

## OPEN SOURCED PROJECTS

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WhereWulff: An Autonomous Workflow to Democratize and Scale Complex Material Discovery for Electrocatalysis

🌐 <https://github.com/ulissigroup/mo-wulff-workflow>

➤ 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.

# RESEARCH CONTRIBUTIONS

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## Publications

- Sanspeur, R., J. Heras-Domingo, and Z. Ulissi (2022). "WhereWulff: An Autonomous Workflow to Democratize and Scale Complex Material Discovery for Electrocatalysis". In: *in preparation*.
- Tran, R., J. Lan, M. Shuaibi, B. Wood, S. Goyal, A. Das, J. Heras-Domingo, A. R. A. Kolluru, N. Shoghi, A. Sriram, Z. Ulissi, and C. Zitnick (2022). "The Open Catalyst 2022 (OC22) Dataset and Challenges for Oxide Electrocatalysis". In: *ArXiv*.
- 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 IrO<sub>2</sub> 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*.
- González, D., J. Heras-Domingo, S. Pantaleone, A. Rimola, L. Rodríguez-Santiago, X. Solans-Monfort, and M. Sodupe (2019). "Water Adsorption on MO<sub>2</sub> (M= Ti, Ru, and Ir) Surfaces. Importance of Octahedral Distortion and Cooperative Effects". In: *ACS Omega* 4 (2).
- 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).
- 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).

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## Conferences Participation

- 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 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 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 Química Teórica i Computacional. 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

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### Teaching (2015/2019) at Autonomous University of Barcelona (UAB)

Total Hours of Teaching: 306.16

Area: Physical Chemistry

Subjects:

- Analysis and Determination of Properties
- Chemical Thermodynamics
- Spectroscopy
- Chemical Reactivity

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### Research Supervision (2015/2019) at Autonomous University of Barcelona (UAB)

Number of Projects: 4

Area: Computational Chemistry for Materials Science

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### Research Supervision (2021/2022) at Carnegie Mellon University (CMU)

Number of Projects: 1

Area: Graph neural networks for transition metal complexes

## REFERENCES

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Prof. Zachary W. Ulissi

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