JAVIER HERAS DOMINGO

Ph.D. in Theoretical Chemistry

07-February-1991

jherasdo@andrew.cmu.edu

https://jherasdo.github.io

orcid.org/0000-0002-4322-3146

https://github.com/jherasdo

EXPERIENCE

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
- Deep Learning for Transition metal Complexes

EDUCATION

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

Autonomous University of Barcelona

January 2016 - January 2020 | Bellaterra Campus, Barcelona (Spain)

- Thesis Title: "Modeling of RuO2 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

- **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

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

Publications

- Sanspeur, R., J. Heras-Domingo, and Z. Ulissi (**2022**). "WhereWulff: An Autonomous Workflow to Democratize and Scale Complex Material Discovery for Electocatalysis". 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 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.
- 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).
- 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).

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 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 (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

Research Supervision (2015/2019) at Autonomous University of Barcelona (UAB)
Number of Projects: 4
Area: Computational Chemistry for Materials Science

Research Supervision (2021/2022) at Carnegie Mellon University (CMU)
Number of Projects: 1
Area: Deep Learning for Transition Metal Complexes

REFERENCES

Prof. Zachary W. Ulissi
Carnegie Mellon University
zulissi@andrew.cmu.edu

Prof. Gabe Gomes
Carnegie Mellon University
gdgomes@andrew.cmu.edu

Prof. Mariona Sodupe
Autonomous University of Barcelona
mariona.sodupe@uab.cat

Prof. Xavier Solans-Monfort
Autonomous University of Barcelona
xavier.solans@uab.cat