JAVIER HERAS DOMINGO

Ph.D. in Theoretical Chemistry

07-February-1991

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EXPERIENCE

Postdoctoral Researcher

Ulissi Group - Carnegie Mellon University

February 2020 - Currently

Pittsburgh, Pennsylvania, USA

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 stay 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)

FURTHER EDUCATION

Deep Learning Nanodegree Program with Pytorch

Udacity

September 2020 - December 2020

Pittsburgh, Pennsylvania, USA

RESEARCH CONTRIBUTIONS

Publications

- Heras-Domingo, J., M. Sodupe, and X. Solans-Monfort (**2018**). "Interaction between ruthenium oxide surfaces and water molecules. Effect of surface morphology and water coverage". In: *The Journal of Physical Chemistry C* 123.13, pp. 7786–7798.
- Gonzalez, D., J. Heras-Domingo, S. Pantaleone, A. Rimola, L. Rodriguez-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, pp. 2989–2999.
- Luis-Barrerra, J., R. Cano, G. Imani-Shakibaei, J. Heras-Domingo, J. Pérez-Carvajal, I. Imaz, D. Maspoch, X. Solans-Monfort, J. Alemán, and R. Mas-Ballesté (**2019**). "Switching acidic and basic catalysis through supramolecular functionalization in a porous 3D covalent imine-based material". In: *Catalysis Science & Technology* 9.21, pp. 6007–6014.

- 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: *The Journal of Physical Chemistry C* 124.1, pp. 1227–1237.
- 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, pp. 1189–1198.
- 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.

Conferences Participation

- 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.
- 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 (**2018**). "From Surface to Nanoparticles: Ruthenium Oxide Systems and their Interaction with water". In: *International Congress of Quantum Chemistry (ICQTC) Congress. Flash Presentation + Poster*. Menton, France.
- 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.

Workshops Assistance

- *Vienna Ab Initio Simulation Package (VASP)* (**2016**). Rennes, France: ICAMM Workshop.
- *Introduction to Statistical Computing in Python* (**2017**). Barcelona, Spain: Servei de Genòmica I Bioinformàtica.
- *Machine Learning for Material Science* (**2019**). Helsinki, Finland: Aalto University.
- *Machine learning: How to coarse-grain* (**2020**). Online: CECAM-DE-SMSM.

TEACHING AND RESEARCH SUPERVISION

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

LANGUAGES

Spanish
Catalan
English
German