Yoshio Alan Torres Barrera

Website YoshioBarrera
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EDUCATION

National Autonomous University of Mexico (UNAM) Mexico City, Mexico
Ph.D. Chemistry September 2020 – November 2024
Thesis: "*Reactivity Prediction in Radical Chemistry: Advances and Applications of General-Purpose Reactivity Indicators*"
Advisor: Dr. James S. M. Anderson

Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV) Merida, Mexico
M.Sc. Physical Chemistry August 2016 - August 2018 Thesis:
"*Structure and Stability of Transition Metal Hydrides with Formula MH_{14} and MH_{15}"*
Advisor: Dr. José Gabriel Merino Hernández

University of Guadalajara (UdeG) Guadalajara, Mexico
B.S. Chemistry January 2011 - June 2015
General Knowledge Exam on Chemistry (CENEVAL): Outstanding

RESEARCH EXPERIENCE

RWTH Aachen University Aachen, Germany
Advanced Research Opportunities Program (AROP) January – June 2025
Project: *"Gauging the Acidity of Doubly Cationic Lewis Acids with Oxide and Fluoride Ion Affinities"*
Advisor: Dr. Florian F. Mulks

McMaster University Ontario, Canada
Visiting Student October – December 2023
Project: "*Different ways to Calculate the Fukui Function*"
Advisor: Dr. Paul W. Ayers

Center for Electrochemical Research (CIDETEQ) Queretaro, Mexico
Visiting Student (Summer Internship) Jun 2014 – Jul 2014
Project: "*Synthesis and Characterization of Yttrium Thin Films*"
Advisor: Dr. Raul Ortega Borges

PUBLICATIONS

4. **Barrera Y.**, Anderson J.S.M., Comparative Study of Predicting Radical C-H Functionalization Sites in Nitrogen Heteroarenes Using a Radical General-Purpose Reactivity Indicator and the Radical Fukui Function, *J. Comput. Chem.* 46 (**2025**) e70130. https://doi.org/10.1002/jcc.70130.
3. **Barrera Y.**, Mulks F.F., Strained diradicaloids for σ-bond-insertion reactions: A breakthrough in drug discovery, *Chem* (**2025**) 102524. https://doi.org/10.1016/j.chempr.2025.102524.

2. **Barrera Y.**, Anderson J.S.M., Does the radical GPRI strongly depend on the population scheme?: Predicting radical attack on unsaturated molecules, *J. Comput. Chem*. 45 (**2024**) 1152–1159. https://doi.org/10.1002/jcc.27314.
1. **Barrera Y.**, Anderson J.S.M., Predicting the reactivity of unsaturated molecules to methyl radical addition using a radical two-parameter general-purpose reactivity indicator, *Chem. Phys. Lett*. 791 (**2022**) 139333. https://doi.org/10.1016/j.cplett.2021.139333.

BOOK CHAPTERS

2. **Barrera Y.**, Kawasaki A., Ayers P.W., Anderson J.S.M., The Ehrenfest force, in: J.I. Rodríguez, F. Cortés-Guzmán, J.S.M. Anderson (Eds.), *Adv. Quantum Chem. Topol. Beyond QTAIM*, 1st ed., Elsevier, **2023**: pp. 225–244. https://doi.org/10.1016/B978-0-323-90891-7.00019-0.
1. **Barrera Y.**, Anderson J.S.M., Predicting reactivity with a General-Purpose Reactivity Indicator, in: S. Kaya, L. VonSzentpaly, G. Serdaroglu, L. Guo (Eds.), *Chem. React. Vol. 2 Approaches Appl.*, 1st ed., Elsevier, **2023**: pp. 159–180. DOI: https://doi.org/10.1016/B978-0-32-390259-5.00012-3.

SUBMITTED PUBLICATIONS and IN-PROGRESS PUBLICATIONS

2. **Barrera Y.**, Mulks F., *Gauging the Acidity of Doubly Cationic Lewis Acids with Oxide and Fluoride Ion Affinities*, **2025**. *In preparation*.
1. **Barrera Y.**, Rocha-Rinza T., Mulks F., Ayers P.W, Anderson J.S.M., The Grand Canonical General-Purpose Reactivity Indicator: A Conceptual DFT Approach to Predict Molecular Reactivity and Experimental Electrophilicity and Nucleophilicity Scales, **2025**. *Submitted*.

PRESENTATIONS

5. **Barrera Y.**, Anderson J.S.M., "*Elucidating radical C-H functionalization on heteroarenes with a radical GPRI*", 20th International Conference on Density Functional Theory and its Applications, École Nationale Supérieure de Chimie, Paris, France, **2024**. *Poster*.
4. **Barrera Y.**, Anderson J.S.M., "*Predicting the most reactive atom in methyl radical addition reactions with the R-GPRI*", Symposium of Institute of Chemistry and CINVESTAV, Mexico City, Mexico, **2024**. *Poster*.
3. **Barrera Y.**, Anderson J.S.M., "*Conceptual DFT models to predict the regioselectivity of molecules under radical attacks*", Farnaz Heidar-Zadeh group meeting, Department of Chemistry, Queen's University, Kingston, Ontario, Canada **2023**. *Presentation*.
2. **Barrera Y.**, Anderson J.S.M., "*Elucidating radical addition reactions using the radical General-Purpose Reactivity Indicator*, Monthly meeting in the Department of Physical Chemistry, Institute of Chemistry, UNAM, Mexico City, Mexico, **2023**. *Presentation*.
1. **Barrera Y.**, Merino G., "*Structure and Stability of Transition Metal Hydrides with Formula MH_{14} and MH_{15}*", XVI Mexican Meeting of Theoretical Chemistry, Puebla, Mexico, **2017**. *Poster*.

INVITED LECTURES

National Autonomous University of Mexico (UNAM) Mexico City, Mexico
Institute of Chemistry Feb – Mar 2022
Course Instructor for Master Degree Aspirants: Thermodynamics and Kinetics Part 1

TEACHIING EXPERIENCE

La UNI Mexico City, Mexico
Biochemistry and Algebra, Bachelor School Sep 2024 – Dec 2024

- I taught Biochemistry in the Odontology school, and Algebra at the computer Science school.

British Institute Zapopan, Mexico
Science Teacher, Secondary School Aug 2019 – Jun 2020

- I taught middle school courses in Biology, Physics and Chemistry with a strong emphasis on experiments.

Technological University of Guadalajara (UTEG) Guadalajara, Mexico
Chemistry Teacher, High School Sep 2018 – Jun 2019

- I taught high school courses in Chemistry.

PROFESSIONAL EXPERIENCE

Belticos S.A. de C.V. Zapopan, Mexico
Quality Assurance Chemist Jul 2015 – Feb 2016

- Conducting quality tests on in-process and finished products in the beverage industry to ensure compliance with industry standards.

SKILLS

- English (TOEFL ITP) = 540 (2023, improving)
- Portuguese (Completed the first four courses at ENALLT, UNAM)
- Density Functional Theory (DFT)
- Molecular Modelling (Gaussian, ORCA, ADF, Quantum Espresso)
- Molecular Visualization (Blender, Chemcraft, VMD, Chemdraw, PyMol, ChimeraX)
- Intermediate in Python
- Beginner level in HTML, CSS and JavaScript

INTERESTS

- Chemical Reactivity
- Quantum Tunneling in Chemistry
- Machine Learning
- Solid State Chemistry