Yoshio Alan Torres Barrera

Websites YoshioBarrera
MyFavoriteMonthlyMolecule
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EDUCATION

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

The Center for Research and Advanced Studies of the National Polytechnic Institute (CINVESTAV) Merida, Mexico
M.Sc. Physical Chemistry 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 June 2015
General Knowledge Exam on Chemistry (CENEVAL): Outstanding (Sobresaliente)

RESEARCH EXPERIENCE INTERNSHIP

McMaster University Ontario, Canada
Visiting Student Oct 2023 – Dec 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

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. DOI: 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. DOI: 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. DOI: 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

3. **Barrera Y.**, Anderson J.S.M., "The Ultimate Condensed-by-Atom Radical Fukui Function: A Computational Benchmark Study", **2024**. *In preparation.*
2. **Barrera Y.**, Anderson J.S.M., Grand-Canonical Ensemble Conceptual Density-Functional Theory to Predict Electrophilicity and Nucleophilicity: Derivation and Test of the Grand Canonical General-Purpose Reactivity Indicator, **2024**. *Submitted*.
1. **Barrera Y.**, Anderson J.S.M., Comparative Study of Predicting Radical C-H functionalization Sites in Nitrogen Heteroarenes Using the Radical General-Purpose Reactivity Indicator and Radical Fukui Function, **2024**. *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 (upcoming August 2024)*.
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

UNID Mexico
Science Teacher, High School Feb – Jun 2024

- Taught high school short courses (60 minutes each, twice a week) covering various topics in Physics and Chemistry.

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

- 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

- 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)
- Conceptual DFT
- Molecular Modelling (Gaussian, ADF, Quantum Espresso)
- Molecular Visualization (Blender, Chemcraft, VMD, Chemdraw, PyMol, ChimeraX)
- Molecular Docking (AutoDock)
- Intermediate in Python
- Intermediate in Fortran
- Beginner level in HTML, CSS and JavaScript (see Websites).

INTERESTS

- Quantum Tunnelling in Chemistry
- Machine Learning
- Solid State Chemistry