

Yoshio Alan Torres Barrera

Websites

[YoshioBarrera](#)

[MyFavoriteMonthlyMolecule](#)

Email

yoshiobarrera@gmail.com

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 GPRF*”, 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-GPRF*”, 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 Heidari-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](#)

TEACHING EXPERIENCE

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