

Alicia Odette Hernandez-Castillo, PhD

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Harvey Mudd College
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Positions

Assistant Professor of Chemistry 07/2022 – present
Harvey Mudd College Claremont, CA, USA

Postdoctoral Research Fellow 11/2018 – 05/2022
Fritz-Haber-Institut der Max Planck-Gesellschaft Berlin, Germany
(*Fritz-Haber-Institute of the Max Planck Society*)
Supervisor: Dr. Sandra Eibenberger-Arias; Director: Prof. Gerard Meijer

Education

Ph.D in Chemistry 08/2014 – 10/2018
Purdue University West Lafayette, IN, USA
Dissertation: “Broadband Microwave Spectroscopy of Lignin, Biofuels, and Their Pyrolysis Intermediates.”
Supervisor: Prof. Timothy S. Zwier.

Master’s in Musical Composition, with honors 08/2012 – 05/2014
Facultad de Música. Universidad Nacional Autónoma de México (FaM – UNAM) Mexico City, Mexico
(*Department of Music, National Autonomous University of Mexico*)

B.S. in Chemistry, with honors 08/2009 – 12/2013
Facultad de Química. Universidad Nacional Autónoma de México (FQ – UNAM) Mexico City, Mexico
(*Department of Chemistry, National Autonomous University of Mexico*)
Thesis: “Simetría y degeneración de una particular en una caja cúbica”
(*Symmetry and Degeneracy of an Impenetrable Cubic Well Potential*)
Supervisor: Dr. Renato Lemus.

B.A. in Piano, public exam summa cum laude 08/2006 – 05/2010
Conservatorio Nacional de Música Mexico City, Mexico
(*National Conservatory of Music*)

Teaching Experience

Harvey Mudd

Chemistry in the Modern World, (CHEM 42)
Chemistry Laboratory, (CHEM 24)
Physical Chemistry: Group Theory, Quantum Chemistry, and Spectroscopy (CHEM 52)
Physical Chemistry Laboratory (CHEM 53)
Advanced Analytical Chemistry (CHEM 114)
Chemistry Seminar (CHEM 199)

Purdue University

General Chemistry, (CHM 11100), **Teaching Assistant**
General Chemistry, (CHM 11500), **Teaching Assistant**

UNAM, Mexico City, Mexico

Algebra for chemists, **Teaching Assistant**
Foundations of Spectroscopy, **Teaching Assistant**

Fellowships and Awards

- Ross Fellowship** (Given to top applicants in the College of Science at Purdue University) 2014-2015
Purdue University
- Becas de Excelencia Académica para Estudios de Posgrado en el Extranjero** 2014
Dirección General de Relaciones Internacionales. Secretaría de Educación Pública.
(*Division of International Relations, Department of Public Education. Mexico.*)
- Summer Internship Report Award, undergrad level.** 2010
Report: Structure Observation of Crystal Polystyrene Fibers by SEM and AFM (2nd place)
DGDC-UNAM (*General Direction of Science Communication*)

Grant Applications

- ACS-PRF-New Investigator:** Structure of Succinimide Derivatives as Models for Oil Dispersants
Submission: 2024
Status: Funded
- NSF-Research in Undergraduate Institutions (RUI):** Seeking a solution to the solution – Spectroscopic studies of anticonvulsants-
(H₂O)_n clusters
Submission: 2023
Status: Not Funded

Research Experience

- Harvey Mudd College** 2022-present
- Design and construction of instrumentation for chirped pulse Fourier transform microwave spectrometer in the 6-18 GHz frequency range.
 - Study of succinimides and maleimides in collaboration with the Crabtree group at UC-Davis using microwave spectroscopy in the 6-18 GHz and the 26-40 GHz frequency ranges.
 - Design and construction of Resonant enhance multiphoton ionization (REMPI) time-of-flight (TOF) mass spectrometer to study molecules in excited electronic states.
 - Analysis of the structures of cyclic ketones and their derivatives using microwave spectroscopy with a particular interest in understanding their large-amplitude motions such as ring-puckering and methyl internal rotation.
- Fritz-Haber-Institut der Max Planck-Gesellschaft** 2018-2022
Postdoctoral research associate in the Department of Molecular Physics, Controlled Molecules Group
Supervisor: Dr. Sandra Eibenberger-Arias; Director: Prof. Gerard Meijer
- Design and construction of instrumentation for UV-microwave multi-resonance methods in the gas phase.
 - Characterization and computer control of microwave components for a chirped-pulse Fourier transform microwave (CP-FTMW) spectrometer.
 - Manipulation of quantum coherences between rotational states to enhance or deplete population in single quantum states and detect state-specific enantiomeric enrichment.
 - High resolution UV studies of chiral molecules.
- Purdue University (Ph.D. Research)** 2014 – 2018
Supervisor: Prof. Timothy S. Zwier.
- Detection and structural characterization of pyrolysis intermediates of potential plant-derived biofuels with microwave spectroscopy (CP-FTMW) and mass spectrometry (TOFMS) using a pyrolysis source coupled to a supersonic expansion.
 - Development of Strong Field Coherence Breaking (SFCB), a conformer/isomer specific microwave technique.
 - Development of a set of MatLab programs to analyze microwave data efficiently. Used C++ to communicate with a state-of-the-art digitizer in order to acquire microwave spectra. Incorporation of protocols to simplify spectral assignments using multi-resonance effects.
 - Designed and implemented modifications to the pyrolysis source and spectrometer that improved the quality and speed of data acquisition.
 - Conformational analysis using laser-induced fluorescence, single-conformation IR measurements, and microwave spectroscopy.

Publications

Chisom A. Dim, Caroline Sorrells, **A. O. Hernandez-Castillo**, Kyle N. Crabtree. “*K_a-Band Rotational Spectroscopy of Succinimide and N-Chlorosuccinimide*”, J. Phys. Chem. A. **128**, 9754 (2024)

Lughnasa York, Caroline Sorrells, Chisom A. Dim, Kyle N. Crabtree, and **A.O. Hernandez-Castillo**. “*A Tale of Two Tails: Rotational Spectroscopy of N-Ethyl Maleimide and N-Ethyl Succinimide*”, J. Phys. Chem. A. **128**, 5541 (2024).

Ju Hyeon Lee, Johannes Bischoff, **A.O. Hernandez-Castillo**, Elahe Abdiha, Boris G. Sartakov, Gerard Meijer, and Sandra Eibenberger-Arias. “*The Influence of microwave pulse conditions on enantiomer-specific state transfer*”, New Journal of Physics. **26**, 033015 (2024)

Ju Hyeon Lee, Johannes Bischoff, **A.O. Hernandez-Castillo**, Boris G. Sartakov, Gerard Meijer, and Sandra Eibenberger-Arias. “*Quantitative study of enantiomer-specific state Transfer*”, Phys. Rev. Lett. **128**, 173001 (2022)

A.O. Hernandez-Castillo, Camila Calabrese, Sean M. Fritz, Iciar Uriarte, Emilio J. Cocinero, and Timothy S. Zwier. “*Bond Length Alternation and Internal Dynamics in Model Aromatic Substituents of Lignin*”, ChemPhysChem **23**, e202100808 (2022)

A.O. Hernandez-Castillo, Johannes Bischoff, Ju Hyeon Lee, Jennifer Langenhan, Mallikarjun Karra, Gerard Meijer, and Sandra Eibenberger-Arias. “*High Resolution UV Spectroscopy of 1-Indanol*”, Phys. Chem. Chem. Phys. **23**, 7048 (2021)

A.O. Hernandez-Castillo, F. Robicheaux, and Timothy S. Zwier. “*Propagating molecular rotational coherences through Single-Frequency Pulses in the strong field regime*” J. Chem. Phys. **151**, 084312 (2019)

Sean Fritz, Brian M. Hays, **A.O. Hernandez-Castillo**, Chamara Abeysekera, and Timothy S. Zwier. “*Multiplexed Characterization of complex Gas-Phase Mixtures Combining Chirped-Pulse Fourier Transform Microwave Spectroscopy and VUV photoionization Time-of-flight Mass Spectrometry*”. Rev. Sci. Instrum. **89**, 0931101 (2018)

Chamara Abeysekera, **A.O. Hernandez-Castillo**, John Stanton, and Timothy S. Zwier. “*Broadband Microwave Spectroscopy of 2-furanyloxy Radical: Primary pyrolysis product of 2-Methoxyfuran*” J. Phys. Chem. A. **122**, 6879 (2018), *ACS Editor's Choice Aug. 19, 2018*

Sean Fritz, **A.O. Hernandez-Castillo**, Chamara Abeysekera, and Timothy S. Zwier. “*Structure Determination of 3-phenylpropionitrile by Strong Field Coherence Breaking*” J. Mol. Spec. **349**, 10 (2018)

A.O. Hernandez-Castillo, Chamara Abeysekera, Brian M. Hays, Isabelle Kleiner, Ha Vinh Lam Nguyen, and Timothy S. Zwier. “*Conformational preferences and internal rotation of Methyl Butyrate by Microwave Spectroscopy*” J. Mol. Spec. **337**, 51 (2017)

A.O. Hernandez-Castillo, Chamara Abeysekera, Brian M. Hays and Timothy S. Zwier. “*Broadband Multi-resonant Strong Field Coherence Breaking as a tool for single isomer microwave spectroscopy*” J. Chem. Phys. **145**, 114203 (2016)

Joseph R. Gord, Daniel M. Hewett, **Alicia O. Hernandez-Castillo**, Karl N. Blodgett, Mathew C. Rotondaro, Adalgisa Varuolo, Matthew A. Kubasik and Timothy S. Zwier “*Conformation-specific spectroscopy of capped, gas phase Aib oligomers: Test of the Aib residue as a 3₁₀-helix former*” Phys. Chem. Chem. Phys., **18**, 25512 (2016)

R. Lemus. and **A.O. Hernández-Castillo** “*Symmetry projection, geometry and choice of the basis*”. Revista Mexicana de Física E. **61**, 113 (2015)

A.O. Hernández-Castillo and R. Lemus. “*Symmetry group of an impenetrable cubic well potential*” J. Phys. A: Math. Theor. **46**, 464201 (2013)

Presentations

77th International Symposium on Molecular Spectroscopy

The University of Illinois at Urbana-Champaign. Urbana, IL, USA, 2024

- *Rotational Spectroscopy of Succinimide Derivatives* (Oral Presentation)

University of New Haven, Invited talk

West Haven, CT, USA, 2023

- *Broadband Microwave Spectroscopy of Highly Functionalized 5-Membered Ring Organic Molecules*

Annual Royal Society of Chemistry Spectroscopy & Dynamics Group Meeting

Virtual conference, 2022

- *Working towards forming an enantiomerically pure rotational state via ESST* (Contributed talk)

Boston College, Invited talk

Virtual Seminar, Newton, MA, USA, 2022

- *Multiplexed Approach to Broadband Rotational Spectroscopy: From Complex Gas Mixtures to Chiral Analysis*

Northwestern University, Invited talk

Evanston, IL, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: From Complex Gas Mixtures to Chiral Analysis*

Indiana University, Invited talk

Bloomington, IN, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: From Complex Gas Mixtures to Chiral Analysis*

Trinity College, Invited talk

Hartford, CT, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: An Ideal Molecular Shape Detector*

Fairfield University, Invited talk

Fairfield, CT, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: An Ideal Molecular Shape Detector*

Wabash College, Invited talk

Crawfordsville, IN, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: An Ideal Molecular Shape Detector*

Hamilton College, Invited talk

Clinton, NY, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: An Ideal Molecular Shape Detector*

Harvey-Mudd College, Invited talk

Harvey-Mudd College, Claremont, CA, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: An Ideal Molecular Shape Detector*

University of Virginia, Rising Star in Chemistry Postdoctoral Seminar Series

Virtual seminar, Charlottesville, VA, USA, 2021

- *Multiplexed Approach to Broadband Rotational Spectroscopy: From Complex Gas Mixtures to Chiral Analysis*

74th International Symposium on Molecular Spectroscopy

Virtual conference, 2021

- *Manipulation of Cold Chiral Molecules Using Electronic and Rotational Spectroscopy* (Oral Presentation)

University of British Columbia, Physical Chemistry Seminar

Virtual seminar, Vancouver, BC, Canada, 2021

- *Broadband Rotational Spectroscopy: From Complex Gas Mixtures to Chiral Analysis*

67th Pacific Conference on Spectroscopy and Dynamics

Bahia Resort, San Diego, CA, USA, 2020

- *Electronic and Rotational Spectroscopy of Cold Chiral Molecules* (Contributed talk and Poster)

Invited talk delivered at the Molecular Physics Dept. Seminar

Fritz-Haber-Institut der Max-Planck-Gesellschaft. Berlin, Germany, 2018

- *Broadband Rotational Spectroscopy as a Tool to Detect & Characterize Pyrolysis Intermediates*

73rd International Symposium on Molecular Spectroscopy

The University of Illinois at Urbana-Champaign. Urbana, IL, USA, 2018

- *Structural Characterization of Phenoxy Radical Using a Mass-Correlated Broadband Microwave Spectrometer* (Oral Presentation)

Purdue University Physical Chemistry Seminar

West Lafayette, IN, USA, 2018

- *Broadband Rotational Spectroscopy as a Tool to Detect & Characterize Pyrolysis Intermediates*

26th Conference on the Dynamics of Molecular Collisions

Granlibakken Conference Center, Tahoe City, CA USA, 2017

- *Using Multi Resonance Effects in Microwave Spectroscopy as a Tool to Characterize Reactive Intermediates* (Hot topics talk and poster)

72nd International Symposium on Molecular Spectroscopy

The University of Illinois at Urbana-Champaign. Urbana, IL, USA, 2017

- *Conformational Study of Dibenzylether* (Oral Presentation)

71st International Symposium on Molecular Spectroscopy

The University of Illinois at Urbana-Champaign. Urbana, IL, USA, 2016

- *Isomer Specific Microwave Spectrum of E- and Z-Phenylvinyl nitrile. Implementing a New Multi-Resonant Spectral Analysis Tool* (Oral presentation)

8th Symposium on Quantum Theory and Symmetries

El Colegio Nacional. Mexico City, Mexico, 2013

- *Symmetry Group of an Impenetrable Cubic Well Potential* (Poster presentation)

XLIII Latin American School of Physics: ELAF 2013

El Colegio Nacional. Mexico City, Mexico, 2013

- *Symmetry Group of an Impenetrable Cubic Well Potential* (Poster presentation)

Professional Development

Fostering a sense of belonging in STEM: The Role of Teaching and Mentoring! 2022
Scripps College

Women in Natural Sciences (WiNS), summer school 2021
Humboldt-Universität
(*Humboldt University*)

- Scientific talks and discussions on light-matter interaction in inorganic, organic, and bio-materials.
- Short workshop on career strategies and personal development.

LabVIEW training workshop 2019
Fritz-Haber-Institut der Max Planck-Gesellschaft
(*Fritz-Haber-Institute of the Max Planck Society*)

- Successfully completed two training courses in National Instruments LabVIEW, where fundamental and advanced skills were discussed.

Presentation Workshop for Female Scientists 2019
Fritz-Haber-Institut der Max Planck-Gesellschaft
(*Fritz-Haber-Institute of the Max Planck Society*)

- Successfully completed a workshop where topics such as gender stereotypes, nonverbal communication (body language), and stage-fright were discussed.

Subprograma 121, Formación de Profesores 2013-2014
Facultad de Química. Universidad Nacional Autónoma de México (FQ – UNAM)
(*Department of Chemistry, National Autonomous University of Mexico*)

- Successfully completed a teaching workshop which included topics such as course/syllabus planning, student assessment, and active learning strategies.
- Acted as a single teaching assistant for two undergraduate courses.

Professional and Scholarly Associations

American Chemistry Society
American Physical Society

Senior thesis students

Natalie Couch 2024
Thesis: Rotational Spectroscopy of Water-Ketone Clusters
Currently: PhD student in chemistry at the University of Colorado Boulder

Laura Wu 2023
Thesis: Assembly of the Electronic Circuit for a Chirped-Pulse Microwave Spectrometer in the 6-18 GHz Region
Currently: PhD student in materials science at Cornell University

Ezra Bacon-Gershman 2023
Thesis: Design and Construction of a Chirped-Pulse Microwave Spectrometer in the 6-18 GHz Region
Currently: PhD student in chemistry at University of Washington

Undergraduate research students

Amir Gonzalez Camacho '26 Research in Chemistry (1 semester) / Summer Research – 2024 - present
Chemistry major
Project: Synthesis and Rotational Spectroscopy analysis of ¹³C Isotopologues in Succinimide.

Huanhuan Huang '27 Research in Chemistry (1 semester) / Summer Research - 2024-present
Engineering major
Project: Rotational spectroscopy of Cyclotene. / Development of a GUI for XIAM.

- Cameron Warmerdam '27** Research in Chemistry (1 semester) / Summer Research – 2024 - present
Physics major
Project: Testing REMPI spectrometer. / Design of Pulse Valve Translator.
- Channing Christian '25** Research in Chemistry (3 semesters) / Summer Research - 2023 - present
Computer Science major
Project: Develop Code to Run REMPI Experiments. / Design and Build Pulse Valve Translator.
- Natchayaporn Sindhurattavej '26** Research in Chemistry (1 semester) - 2024
Chemistry major
Project: Testing REMPI spectrometer.
- Tatiana Cardoso '26** Research in Chemistry (3 semesters) - 2023-2024
Chemistry major
Project: Rotational Spectroscopy of Cyclic Ketones
- Luna York '26** Research in Chemistry (3 semesters) / Summer Research - 2022-2024
Computer Science major
Project: Rotational Spectroscopy of Succinimide and its Derivatives
- Caroline Sorrells '26** Research in Chemistry (3 semesters) / Summer Research - 2022-2023
Physics major
Project: Rotational Spectroscopy of Succinimide and its Derivatives
- Leah McCarthy '25** Research in Chemistry (1 semester) - 2023
Physics major
Project: Design and construction of REMPI spectrometer.
- Jee-In Kwon '25** Summer research - 2023
Physics major
Project: Design and construction of REMPI spectrometer.
- Diane Park '26** Summer research - 2023
Computer Science major
Project: Design and construction of REMPI spectrometer.
- Elena Williams '25** Research in Chemistry (2 semesters) - 2022
Physics major
Project: Testing the Horn Antennas of our Microwave Spectrometer / Building the Mounts for the Horn Antennas
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