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**

Professional and Scholarly Associations

American Chemistry Society
American Physical Society

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*)

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 succinimide 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 the electronic state.
- Analysis of ketone containing molecules with microwave spectroscopy with a particular interest in understanding the low amplitude motions such as puckering motions 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 spectroscopic data. 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, and microwave spectroscopy.

Publications

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 sate 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 3_{10}-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*

74nd 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*

73nd 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-Phenylvinylnitrile. Implementing a New Multi-Resonant Spectral Analysis Tool* (Oral presentation)

8-th 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.

Senior thesis students

Natalie Couch 2024
Thesis: Rotational Spectroscopy of Water-Ketone Clusters

Laura Wu 2023
Thesis: Assembly of the Electronic Circuit for a Chirped-Pulse Microwave Spectrometer in the 6-18 GHz Region

Ezra Bacon 2023
Thesis: Design and Construction of a Chirped-Pulse Microwave Spectrometer in the 6-18 GHz Region

References

- Prof. Dr. Gerard Meijer, Director of the Department of Molecular Physics. *Fritz-Haber-Institute (FHI) of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin*. Phone: +49-30-8413-5602, Email: meijer@fhi-berlin.mpg.de.
- Dr. Sandra Eibenberger-Arias, Group Leader at the Department of Molecular Physics. *Fritz-Haber-Institute (FHI) of the Max-Planck-Society, Faradayweg 4-6, D-14195 Berlin*. Phone: +49-30-8413-5736, Email: eibenberger@fhi-berlin.mpg.de.
- Prof. Dr. John F. Stanton, Department of Chemistry, University of Florida. *214 Leigh Hall, P.O. Box 117200, Gainsville, FL, 32611*. Phone: +1-512-293-9622, Email: johnstanton@ufl.edu.
- Prof. Dr. Brooks H. Pate, Department of Chemistry, University of Virginia, *McCormick Road, P.O. Box 400319, Charlottesville, VA, 22904-4319*. Phone: +1 434-243-0384, Email: bp2k@virginia.edu.
- Dr. Timothy S. Zwier, Principal Scientist, Combustion Research Facility, Sandia National Laboratories. *7011 East Ave., Livermore, CA, 94550*. Phone: +1-925-294-3358, Email: tszwier@sandia.gov.