

# Alicia Odette Hernandez-Castillo, PhD

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**Harvey Mudd College**  
 Department of Chemistry  
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## Profile

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Physical chemist with experience in molecular spectroscopy and advanced instrumental methods. Experienced with microwave electronics, laser systems, fast electronics and state-of-the-art techniques to perform spectroscopic measurements.

## Positions

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**Assistant Professor** 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

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**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

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### Purdue University

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

- Led recitations and laboratory sessions covering general chemistry topics for students not in the college of science.

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

- Led recitations and laboratory sessions covering topics in the beginning principles of first-year general chemistry for undergraduate engineering/science majors.

### UNAM, Mexico City, Mexico

Algebra for chemists, **Teaching Assistant**

- Held office hours, assisted in grading, and helped write exercises for a group of over 100 freshman chemistry majors covering topics ranging from a review of high school algebra to an introduction to linear algebra and group theory.

Foundations of Spectroscopy, **Teaching Assistant**

- Held office hours, assisted in grading and teaching, and helped write online problem sets for an undergraduate course covering topics in quantum mechanics and spectroscopy.

## Research Experience

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### 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.

### ICN-UNAM; *Institute of Nuclear Sciences* (Undergraduate Research)

2011-2014

Supervisor: Dr. Renato Lemus.

- Symmetry Group of an Impenetrable Cubic Well Potential

### IF-UNAM; *Institute of Physics* (Summer Research Internship)

2010

Advisor: MSc. Gabriel Morales.

### INNN; *National Institute of Neurology and Neurosurgery* (Summer Research Internship)

2007

Advisor: Dr. Tessy Lopez.

## Technical Skills

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**Data analysis:** Analysis of high-resolution rotation and rotation-vibronic spectra (SPCAT/SPFIT, XIAM, PGOPHER), usage of molecule visualization programs (ChemDraw, Avogadro, GaussView), experience developing programs in Matlab and python to facilitate and expedite spectral analysis.

**Computer skills:** AutoCAD, Affinity Designer, Adobe Illustrator, OriginPro, Igor Pro.

**Computational chemistry software:** Gaussian, Molpro.

**Programming languages:** C, C++, Python, MatLab, MathCad, LabVIEW.

**Other skills:** RF and microwave electronics, electronic structure calculations, vacuum hardware, laser systems (pulsed dye lasers, Nd-YAG lasers, high power frequency-quadrupled diode lasers, and IR OPO systems), time-of-flight (TOF) mass spectrometry.

**Languages:** Spanish (native), English (fluent), French (fluent), German (intermediate)

## Publications

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Ju Hyeon Lee, Johannes Bischoff, **A.O. Hernandez-Castillo**, Boris 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)

**A.O. Hernandez-Castillo**, Chamara Abeysekera, John F. Stanton, and Timothy S. Zwier. “Structural characterization of Phenoxy Radical with Mass-Correlated Broadband Microwave Spectroscopy” J. Phys. Chem. Lett. **10**, 2919 (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<sub>10</sub>-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

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### 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*

**74<sup>th</sup> 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*

**67<sup>th</sup> 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*

**73<sup>rd</sup> 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*

**26<sup>th</sup> 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)

**72<sup>nd</sup> International Symposium on Molecular Spectroscopy**

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

- *Conformational Study of Dibenzylether* (Oral Presentation)

**71<sup>st</sup> 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)

**8<sup>th</sup> 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**

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**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.

**Fellowships and Awards**

**Ross Fellowship** (Given to top applicants in the college of science at Purdue University)  
Purdue University

2014-2015

**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 (2<sup>nd</sup> place)

DGDC-UNAM (General Direction of Science Communication)

**Departmental and Professional Service****Phi Lambda Upsilon, National Honorary Chemical Society**

Purdue University

- Participated in acquiring funds to support organization goals and events.

**National Chemistry Week**

Purdue University

- Volunteered to guide young audiences through chemistry hands-on experiments and interactive scientific demonstrations.

**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](mailto: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](mailto:eibenberger@fhi-berlin.mpg.de).
- Prof. Dr. John F. Stanton, Department of Chemistry, University of Florida. *214 Leigh Hall, P.O. Box 117200, Gainesville, FL, 32611*. Phone: +1-512-293-9622, Email: [johnstanton@ufl.edu](mailto: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](mailto: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](mailto:tszwier@sandia.gov).