

Mallory Green (Theis), Ph.D.

Curriculum Vitae

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CURRENT POSITION

Postdoctoral Researcher

September 2020 – Present

Fritz Haber Institute, Molecular Physics Department, Berlin, Germany

Current Project:

- ◆ Photoelectron circular dichroism of chiral anions
- ◆ Accepted Beamtime Proposal: Comparative study of the PECD in deprotonated anions, dehydrogenated radicals, and closed-shell neutrals
 - In collaboration with DESIRS beamline of the SOLEIL Synchrotron

Director: Prof. Gerard Meijer, Dr.

External Funding: Alexander von Humboldt Stiftung

EDUCATION

Doctor of Philosophy, Chemistry

May 2020

Emory University, Atlanta, Georgia, USA

Dissertation: “Explorations of beryllium-containing anions through photoelectron velocity map imaging spectroscopy”

Advisor: Dr. Michael Heaven

Bachelor of Science, Chemistry, *magna cum laude*

May 2014

Georgia Southern University, Statesboro, Georgia, USA

Honors Thesis: “Dipole bound states of polycyclic aromatic hydrocarbons containing nitrogen and their relation to the interstellar medium”

Advisor: Dr. Ryan Fortenberry

FELLOWSHIPS AND AWARDS

Miller Prize

June 2023

76th International Symposium on Molecular Spectroscopy

2023 CAS Future Leaders

April 2023

CAS : Division of the American Chemical Society

Alexander von Humboldt Postdoctoral Research Fellowship

December 2021 – December 2023

Alexander von Humboldt Foundation

Quayle Outstanding Dissertation Award

May 2020

Department of Chemistry, Emory University

Reaxys PhD Prize 2019 Finalist

October 2019

Elsevier Solutions

Inaugural Quayle Advanced Scholar Teaching Fellowship

August 2019 – December 2019

Department of Chemistry, Emory University

FELLOWSHIPS AND AWARDS (cont.)

- Laney Graduate Student Fellowship** August 2015 – May 2020
Laney Graduate School, Emory University
- Honors College Scholarship** August 2010 – May 2014
Honors College, Georgia Southern University

RESEARCH EXPERIENCE

Fritz Haber Institute, Department of Molecular Physics September 2020 – Present
Alexander von Humboldt Postdoctoral Researcher December 2021 – December 2023

Project: Photoelectron circular dichroism of chiral anions

- ◆ Combined position sensitive detection and photoelectron detachment by circularly polarized light, to distinguish anions of chiral enantiomers in the gas phase.
 - Relevant Skills: chiral discrimination, plasma entrainment, photoelastic modulation
- ◆ Employed semi-empirical computational methods (i.e. density functional theory) to assign the energy-resolved electron detachment channels.

Emory University, Department of Chemistry August 2015 – July 2020
Postdoctoral Researcher May 2020 – July 2020
Graduate Researcher August 2015 – April 2020

Project: Understanding bonding in beryllium-containing anions via photoelectron velocity map imaging spectroscopy.

- ◆ Used photoelectron velocity map imaging spectroscopy to analyze previously underexplored, small beryllium-containing molecules in the gas phase.
 - Relevant Skills: high-vacuum systems, pulsed ns UV-nIR lasers, charged particle optics, electron imaging, time-of-flight mass spectrometry, laser ablation
- ◆ Employed computational techniques (including Molpro, Gaussian, Multiwfn) to model spectroscopic information for various molecules.

Georgia Southern University, Department of Chemistry September 2013 – May 2015
Research Scientist May 2014 – May 2015
Undergraduate Researcher September 2013 – April 2014

Project: Dipole bound states of polycyclic aromatic hydrocarbons and their relation to the interstellar medium.

- ◆ Used *ab initio* computational methods (PSI4, CFOUR, Gaussian, EOM-CCSD) to calculate the energies of possible dipole bound and valence bound polycyclic aromatic hydrocarbon anions, which may be present in the interstellar medium.

Nemours Children's Health of Jacksonville, Florida June – July 2012
Summer Intern

Projects:

1. Quality of life in adolescent boys with idiopathic short stature: Positive impact of growth hormone and aromatase inhibitors
2. A randomized, double blind, placebo-controlled pilot trial of the safety and efficacy of atorvastatin in children with elevated low-density lipoprotein cholesterol (LDL-C) and type 1 diabetes
 - ◆ Conducted data management for two clinical trials.
 - ◆ Assisted in coordination of trial patient visits, including organizing laboratory results, and preparing rooms for treatment.

TEACHING / MENTORSHIP EXPERIENCE

Fritz Haber Institute**Graduate Research Supervisor****September 2020 - Present**

- ◆ Direct supervisor of an incoming PhD student and active member of the student's thesis advisory committee.
- ◆ Supervise the dissertation work of a senior PhD student and act as the intermediary between the student and the department director. Dissertation has been submitted for external review.

IMPRS Hand-On Block Course Workshop Instructor**September 2023**

- ◆ Developed a hands-on workshop on ion generation and mass spectrometry for IMPRS PhD students, as part of their required education.

Emory University**Instructor of Record**, CHEM 150: Structures and Properties**Fall Semester 2019**

- ◆ Instructed a class of 55 undergraduate students in the foundations of chemistry, including topics covered in general, organic, inorganic and physical chemistry, as a part of the Department of Chemistry's, "Chemistry Unbound" curriculum.
- ◆ Participated in the semester's curriculum development meeting, where all teaching faculty from both campuses met to refine the full undergraduate curriculum.

Teaching Assistant, PHYS CHEM 2: Thermodynamics & Kinetics**Spring Semester 2017**

- ◆ Provided supplementary instruction and grading assistance for an undergraduate course in thermodynamics and kinetics.

Teaching Assistant, PHYS CHEM 2: Thermodynamics & Kinetics (Laboratory)**Spring Semester 2016**

- ◆ Supervised the laboratory activities of undergraduate students, specifically, provided guidance with a molecular dynamic simulation of protein docking exercise.

Teaching Assistant, PHYS CHEM 1: Quantum Chemistry**Fall Semester 2015**

- ◆ Provided supplementary instruction and grading assistance for an undergraduate course in quantum mechanics

Graduate Research Mentor**Fall 2016 – July 2020**

- ◆ Managed 4 undergraduate research students, 1 BS educated research assistant, and 1 first year graduate student.
- ◆ Created an [introductory guide](#) to computational chemistry for new graduate students and upperclassmen undergraduate students.

Georgia Southern University**Assistant Lab Instructor**, Physical Chemistry 1 & 2 Laboratory**August 2014 – May 2015**

- ◆ Prepped, instructed and graded for all physical chemistry laboratory sections, summing to 45 students per semester.
- ◆ Created a preparatory and instruction guide for future physical chemistry lab instructors.

Research Mentor**January 2014 – May 2015**

- ◆ Supervised 3 undergraduate research students.

Academic Success Center Math and Science Tutor**January 2012 – December 2013**

- ◆ Provided tutoring in subjects including chemistry (general, organic, analytical, physical), biology, physics, calculus, and statistics in an on-campus tutoring center.

PUBLICATIONS

J. Triptow, G. Meijer, A. Fielicke, **M.L. Green***. “Imaging Photoelectron Circular Dichroism in the Detachment of Mass-Selected Chiral Anions” *Angew. Chem. Int. Ed.* **2022** DOI: 10.1002/anie.202212020

J. Triptow, G. Meijer, A. Fielicke, O. Dopfer, **M.L. Green***. “A Comparison of the Conventional and Non-conventional Hydrogen Bond Donors in Au⁻ Complexes.” *J. Phys. Chem. A* **2022**, 126, 24, 3880–3892 DOI: 10.1021/acs.jpca.2c02725

M. L. Green, N. Jaffe and M.C. Heaven. “Characterization of the Ground States of BeC₂ and BeC₂⁻ via Photoelectron Velocity Map Imaging Spectroscopy.” *J. Phys. Chem. Lett.* **2020** 11, 1, 88-92 DOI: 10.1021/acs.jpcllett.9b03297

M. L. Green, Pearl Jean, and Michael C. Heaven. “Dative Bonding between Closed-Shell Atoms: The BeF⁻ Anion” *J. Phys. Chem. Lett.* **2018** 9 (8), 1999-2002 DOI: 10.1021/acs.jpcllett.8b00784

A. R. Dermer, **M. L. Green**, K. J. Mascariolo, and M. C. Heaven. “Photoelectron Velocity Map Imaging Spectroscopy of the Beryllium Sulfide Anion, BeS⁻” *J. Phys. Chem. A* **2017** 121 (30), 5645-5650 DOI: 10.1021/acs.jpca.7b04894

K. J. Mascariolo, A. R. Dermer, **M. L. Green**, A. M. Gardner, M. C. Heaven. “Photodetachment Spectroscopy of the Beryllium Oxide Anion, BeO.” *J. Chem. Phys.* **2017**, 146, 054301–054301, 10.1063/1.4974843

M. L. Theis, A. Candian, A. G. G. M. Tielens, T. J. Lee, and R. C. Fortenberry “Electronically Excited States of Anisotropically Extended Singly-Deprotonated PAH Anions” *J. Phys. Chem. A* **2015**, 11,9 (52), 13048-13054 DOI: 10.1021/acs.jpca.5b10421

M. L. Theis, A. Candian, A. G. G. M. Tielens, T. J. Lee, and R. C. Fortenberry “Electronically Excited States of PANH Anions” *Phys. Chem. Chem. Phys.* **2015**, 17, 14761-14772 DOI: 10.1039/C5CP01354B

* Indicates corresponding author

PEER REVIEW PARTICIPATION

Journal of Physical Chemistry Letters, ACS

Chemistry- A European Journal, Wiley

INVITED PRESENTATIONS

M.L. Green. “Positive outlooks on imaging photoelectron circular dichroism in negatively-charged chiral molecules.” Photon Science Seminar. SLAC National Accelerator Laboratory. Menlo Park, CA, USA, August 15, 2023.

J. Triptow, G. Meijer, A. Fielicke, **M.L. Green**. “Imaging the photoelectron circular dichroism in the photodetachment of deprotonated 1-indanol anion” Department of Physics, University of Kassel, Kassel, Germany, October 17, 2022.

M.L. Green. “A picture worth a thousand data points: Velocity map imaging spectroscopy.” Seminar Series of the Department of Chemistry of Georgia Southern University, Statesboro, Georgia (virtual), January 22, 2021.

M.L. Green, M.C. Heaven. “Explorations of beryllium bonding through photoelectron velocity map imaging spectroscopy.” Molecular Physics Department of the Fritz Haber Institute, Berlin, Germany, February 28, 2020.

ORAL PRESENTATIONS

J. Triptow, V. Brandt, G. Meijer, A. Fielicke, **M.L. Green**. “Imaging the photoelectron circular dichroism in chiral anions” *Proceedings of the 2023 American Chemical Society Fall National Meeting*, San Francisco, CA, USA, August 13-17, 2023.

J. Triptow, V. Brandt, G. Meijer, A. Fielicke, **M.L. Green**. “imaging the photoelectron circular dichroism in the photodetachment of chiral anions” *Proceedings of the 33rd International Symposium on Chirality*, Sapienza Università, Rome, IT, July 24-27, 2023.

J. Triptow, G. Meijer, A. Fielicke, **M.L. Green**. “Imaging the photoelectron circular dichroism in the photodetachment of chiral anions” *Proceedings of the 76th International Symposium on Molecular Spectroscopy*, University of Illinois, Urbana-Champaign, IL, USA, June 19-23, 2023. [**Miller Prize recipient**]

J. Triptow, G. Meijer, A. Fielicke, **M.L. Green**. “Imaging the photoelectron circular dichroism in the photodetachment of deprotonated 1-indanol anion” *Proceedings of the 7th Vibrational Optical Activity conference*, University of Alberta, Edmonton, Canada, August 7-11, 2022.

J. Triptow, G. Meijer, **M.L. Green**. “Can photoelectron circular dichroism work for anions?” *Proceedings of the 75th International Symposium on Molecular Spectroscopy*, virtual, June 21-25, 2021.

M.L. Green, N. Jaffe, M.C. Heaven. “Understanding the chemistry of beryllium-containing triatomic anions, BeX_2^- ($X=\text{C}, \text{O}$), using photoelectron velocity map imaging and ab initio methods.” *Proceedings of the 50th High Resolution Molecular Spectroscopy Colloquium*, Dijon, France, August 25-30, 2019.

M.L. Green, N. Jaffe, M.C. Heaven. “Photoelectron velocity map imaging spectroscopy of Be-containing triatomic anions, BeX_2^- ($X=\text{C}, \text{O}$).” *Proceedings of the 74th International Symposium on Molecular Spectroscopy*, Urbana-Champaign, IL, June 16-20, 2019.

M. L. Green, M. C. Heaven. “Understanding bonding in small beryllium containing ions.” *Proceedings of the 256th American Chemical Society National Meeting and Exposition*, Boston, MA, August 19-23, 2018.

M. L. Theis, P. Jean, M. C. Heaven. “Discovery of dative bonding of beryllium fluoride anion by photoelectron VMI spectroscopy.” *Proceedings of the 73rd International Symposium on Molecular Spectroscopy*, Urbana-Champaign, IL, June 18-22, 2018.

A. R. Dermer, **M. L. Theis**, K. Mascariolo, M. C. Heaven. Photoelectron velocity map imaging of BeS^- . *Proceedings of the 72nd International Symposium on Molecular Spectroscopy*, Urbana-Champaign, IL, June 19-23, 2017.

M. L. Theis, A. Candian, A. Tielens, T. J. Lee, R. C. Fortenberry. “Multiple excited states of PANH anions using informed orbital descriptions.” *Proceedings of the 249th American Chemical Society National Meeting and Exposition*, Denver, CO, March 22-26, 2015.

POSTER PRESENTATIONS

M.L. Green. “Imaging photoelectron circular dichroism in mass-selected chiral anions.” *CAS Future Leaders Workshop* at CAS Headquarters, Columbus, OH, USA, August 7-12, 2023.

M.L. Green, P. Jean, M.C. Heaven. “Dative bonding between closed-shell atoms: The BeF^- anion.” *Reaxys PhD Prize Symposium*, Amsterdam, Netherlands, October 3-4, 2019. [[Poster](#)]

M. L. Theis, A. Candian, A. Tielens, T. J. Lee, R. C. Fortenberry. “Excited states of PAH and PANH anions using informed orbital descriptions.” *Proceedings of the Southeastern Theoretical Computational Association Meeting*, Orlando, FL, May, 2015.

POSTER PRESENTATIONS (cont.)

M. L. Theis, A. Candian, A. Tielens, T. J. Lee, R. C. Fortenberry. "Multiple excited states of PANH anions using informed orbital descriptions." *Proceedings of the Southeastern Theoretical Computational Association Meeting*, Emory University, Atlanta, GA, May, 2014.

M. L. Theis, A. Candian, A. Tielens, T. J. Lee, R. C. Fortenberry. "Multiple excited states of PANH anions using informed orbital descriptions." *Proceedings of the 247th American Chemical Society National Meeting and Exposition*, Dallas, TX, March 16th-20th, 2014.

LEADERSHIP EXPERIENCE

Molecular Physics Journal Club, Molecular Physics Dept, FHI **January- May 2023**
Co-Host

- ◆ Co-hosted a department journal club aimed towards introducing young researchers to seminal papers in different fields and explaining the underlying scientific techniques that drove the article's importance.

75th International Symposium on Molecular Spectroscopy **June 2021**
Session Chair

- ◆ Session Title: "Electronic Structure and Potential energy surfaces"

Rao Prize Judge

- ◆ The Rao Prize is awarded to 3 graduate students each year to recognize outstanding science in spectroscopy, and quality presentation of said science.

WorldWide Working Group seminar series, Molecular Physics Dept, FHI **April – June 2021**
Interim Host

- ◆ Assumed hosting responsibilities for a weekly internal department seminar series for students to introduce them to internationally renowned research groups.

Emory Chemistry Department Recruitment **January 2016 – May 2020**
Student Recruitment

- ◆ Held an organizational role in the preparation of the department's yearly recruitment weekend. Tasks included recruitment materials design, student mentorship, housing tour development, evening activity organization, and acting as host for seminars.

Faculty Recruitment

Acted as a student liaison for new faculty during their recruitment visits by providing support and hosting lunches with the recruited faculty and current graduate students.

Pi Alpha Chemical Society, Emory University **May 2018 – May 2019**
Vice President of Social Affairs

- ◆ Organized social events (once a month), including networking events with alumni, for over 100 graduate students

President **December 2015 – May 2017**

- ◆ Managed my graduate student peers in organizing social, outreach and volunteer activities for graduate student of the Emory Chemistry department.

Emory THANKS Donor Appreciation Event, Emory University **November 2018**
Host

- ◆ Managed event where students wrote thank you cards for program donors.

256th American Chemical Society National Meeting **August 2018**
Invited Discussion Leader

- ◆ Led a discussion and provided advice for undergraduate students considering pursuing a PhD in a session called, "The Graduate School Experience: What to Expect."

BROAD SCIENCE COMMUNICATION ACTIVITIES

Audience Based Science Communication

October 2022 – Present

Coach

- ◆ I meet with group leaders of the Fritz Haber Institute, 1-on-1, to coach them on directed science communication, utilizing audience assessment techniques in construction of their scientific presentations.

How to Deliver an Effective Elevator Pitch

November 2022

Host

- ◆ Developed and hosted a department seminar geared towards helping scientists learn the skills need to deliver an effective elevator pitch.
- ◆ The workshop provided generalized information, to enable the participants to adapt their pitches depending on their audience.

Technical Taboo

Fall 2018 – Spring 2017

Co-creator/ Host

- ◆ A SciCom [video](#) where we ask graduate students to explain their research in under a minute, without using technical language, as designated by their lab mates.
- ◆ Live show was hosted during a department recruitment weekend, where students and professors went head to head to see who could make their research more relatable.

Fluorescence Demo Set

September 2017

Creator

- ◆ Created a set of 4 fluorescence demos to explain basic concepts of spectroscopy to a general audience.
- ◆ Demos can be adapted for school ages K-12, and are low hazardous waste and low cost.
- ◆ Demos have been used by various college groups at numerous science outreach events.

Laser Maze

March 2016

Creator

- ◆ Created a table top optical setup where participants must set up mirrors along a designated path to get a laser beam to hit a target.
- ◆ The game teaches the basics of laser optics and optical safety to a general public.
- ◆ The game is used in a larger Chemistry Carnival event hosted every year in Atlanta, GA.

Science Demonstrations around Atlanta

2015-2020

Volunteer

- ◆ Conducted numerous science demos (fluorescence, chromatography, acid/base chemistry, magnetism, chemical reactions, etc.) for a wide range of ages (kindergarteners up to adults) at various schools and museums around Atlanta, GA.

PROFESSIONAL DEVELOPMENT

CAS Future Leaders Workshop

August 2023

- ◆ Spent a week at the CAS Headquarters learning about company infrastructure, science communication, coaching, scientific enterprise, etc.

Building and Managing Your Research Group Virtual Workshop

May 2023

- ◆ Learned about different leadership styles and strategies for leading a research group. Workshop was geared for senior postdocs and new group leaders.

LabVIEW Training Course

September 2021

- ◆ Certified in “Fundamentals and Practical Experience”

PROFESSIONAL DEVELOPMENT (cont.)

Women in Natural Sciences (WiNS) Summer School

June 2021

- ◆ “Light, matter, and life: Why do we see what we see and how do we understand it?”

ComSciCon Workshop

March 2018

- ◆ Developed verbal/written skills to better communicate scientific concepts.

PROFESSIONAL AFFILIATIONS

American Chemical Society

July 2023

CAS Future Leaders Network

April 2023

Alexander von Humboldt Foundation Network

December 2021

Reaxys Prize Club

October 2019

*CV last updated September 2023