

# Katherine J. Oosterbaan

[kjoosterbaan@gmail.com](mailto:kjoosterbaan@gmail.com)

Berkeley, CA

## EDUCATION

*The University of California, Berkeley*, Berkeley, CA

PhD Candidate in Theoretical Chemistry

Designated Emphasis, Computational and Data Science and Engineering

Advisor: Martin Head-Gordon

August 2016-Present

*The University of Chicago*, Chicago, IL

B.S. in Chemistry with Honors (3.7/4.0 GPA)

Minor in Slavic Languages and Literatures – Czech

Honors Thesis: “Two Methods for Potential Use in Water Purification”

2012-2016

Berkeley Coursework: CHEM 220A Thermodynamics and Statistical Mechanics; CHEM 221A-221B Advanced Quantum Mechanics 1-2; COMPSI C267 Applications of Parallel Computers; CS61A Structure and Interpretation of Computer Programs; CS61B Data Structures; NE C285 Nuclear Security

Relevant Undergraduate Coursework: CHEM 261-263 Quantum Mechanics, Thermodynamics, Chemical Kinetics/Dynamics; CHEM 267 Experimental Physical Chemistry; CHEM 268 Computational Chemistry and Biology; CHEM 201-202 Inorganic Chemistry 1-2; CHEM 230-232 Honors Organic Chemistry; CHEM 233 Intermediate Organic Chemistry; CHEM 121-123 Honors General Chemistry; MATH 152-153 Calculus 2-3; MATH 200-201 Math Methods for the Physical Sciences; PHYS 131-133 Mechanics, Electricity & Magnetism, Waves, Optics & Heat

## RESEARCH EXPERIENCE

*Graduate Student Researcher*, Martin Head-Gordon Group, UC Berkeley

October 2016-Present

- Conducting electronic structure research into a novel method of simulating core excitations in molecules by improving on configuration interaction singles (CIS) theory
- Actively developing code for in-house software package, Q-Chem
- Participating in an experimental collaborations with various UCB groups to identify unknown x-ray spectroscopic peaks
- Selected to initiate and manage group Twitter account, @mhg\_group

*Research Assistant*, Sibener Group, UChicago

January 2014-June 2016

- Created block copolymers with consistent and uniform standing cylinders that can be removed by UV radiation to create porous polymers for applications in water purification
- Performed kinetics study on a metallic catalyst (titania) in both UV and non-UV conditions in order to determine efficacy of its decomposition of common organic contaminants in water
- Learned how to use scanning tunneling microscope (STM) and atomic force microscope (AFM), as well as various methods of depositing polymers and vacuum techniques

Summer Intern, NASA Glenn Research Center (GRC), Cleveland, OH

June-August 2014

- Accepted into highly selective program to assist with the development of more commercially viable organic polymer aerogels (next generation insulation that NASA is hoping to use in EVA suits as well as for lighter-weight planes and spaceships)
- Independently synthesized first ever poly(amide-*b*-ester)-based aerogels and worked with mentor to perform a property optimization study for different ratios of polyamide and polyester with the goal of determining the strongest, most flexible aerogel possible
- Selected to be the only collegiate technical grader for GRC high school intern final project presentations

Research Assistant, Kay Laboratory, UChicago

December 2012-June 2013

- Set up, performed, and documented experiments that tested olfactory capabilities in rodents using custom-built electrical interfaces
- Made judgments on equipment status when running experiments and learned hybrid programming language

## PUBLICATIONS

“Non-orthogonal configuration interaction with single substitutions for the calculation of core excited states: An extension to doublet radicals,” K. J. Oosterbaan, A. F. White, and M. Head-Gordon. *J. Chem. Theor. Comput.* **15**, 2966 (2019).

“Tracing the 266 nm-induced radical formation in dimethyl disulfide using time-resolved X-ray absorption spectroscopy,” K. Schnorr, A. Bhattacharjee, K. J. Oosterbaan, M. Delcey, Z. Yang, T. Xue, A. R. Attar, A. S. Chatterley, M. Head-Gordon, S. R. Leone, and O. Gessner. *J. Phys. Chem. Let.* **10**, 1382 (2019).

“Non-orthogonal configuration interaction with single substitutions for the calculation of core excited states,” K. J. Oosterbaan, A. F. White, and M. Head-Gordon. *J. Chem. Phys.* **149**, 044116 (2018).

## POSTERS AND PRESENTATIONS

“Non-orthogonal configuration interaction with single substitutions for the calculation of core excited states,”

- Molecular Quantum Mechanics Conference, Heidelberg, Germany (July 2019), poster
- West Coast Theoretical Chemistry Symposium, Stanford, CA (March 2018), poster
- Graduate Research Conference, Berkeley, CA (March 2018), presentation

“Two Methods for Potential Use in Water Purification,”

- Undergraduate Honors Thesis Seminars, Chicago, IL (April 2016), presentation

“Synthesis of Poly(amide-*b*-ester)-Based Aerogels,”

- Chicago Area Undergraduate Research Symposium, Chicago, IL (April 2015), poster
- Midstates Consortium for Math and Science Undergraduate Research Symposium, St. Louis, MO (October 2014), poster
- Northeast Ohio Undergraduate Research Symposium, Kent, OH (August 2014), poster

## RELEVANT PROFESSIONAL EXPERIENCE

Member, Science and Arts Academy (SAA) Board of Trustees, Des Plaines, IL

August 2018-Present

- Elected as the first ever alumna board member
- Attend board meetings remotely and in person, and help with planning Board initiatives
- Served as a member of the Excellence In Gifted Education Strategic Work Group for the 2018 strategic planning initiative

*Graduate Student Instructor (GSI) for Chem 120A, UC Berkeley* Spring Semester 2019

- Selected to help instruct for undergraduate quantum mechanics (Chem 120A) taught by Professor Martin Head-Gordon, served as head GSI
- Took lecture notes to be posted for the class, and held office hours and discussion sections, provided feedback to the professor on homework assignments and exams
- Managed administrative aspects of the course, including room reservations, grading homework assignments, and proctoring and grading exams

*Graduate Student Instructor (GSI) for Chem 1A, UC Berkeley* Fall Semester 2016, 2017

- Selected to help instruct a special flipped-classroom section of general chemistry (Chem 1A) for students from underprivileged educational backgrounds, taught by Professor Angelica Stacy
- Facilitated collaborative group work and independent learning during class time and held office hours during the week
- Managed administrative aspects of the course, including grading and uploading homework assignments and proctoring and grading exams

*Core and CAAP General Chemistry Tutor, UChicago* School Year 2015-2016

- Assisted general chemistry students with problem solving skills and understanding concepts in general chemistry
- As a CAAP (Chicago Academic Achievement Program) tutor, assisted students from underprivileged academic and socioeconomic backgrounds in adjusting to college-level chemistry

*Collaborative Learning in Chemistry Team Leader, UChicago Department of Chemistry* School Years 2013-2015

- Selected based on academic and leadership potential to lead weekly collaborative problem-solving sessions for General Chemistry students
- Planned weekly approach with other team leaders, ensured group cohesion while facilitating students' independent learning during class, and documented challenges and successes after each session

*Marketing Intern, Abbott Laboratories (Nutrition International Division)* June-September 2013

- Created the international website and related materials, including clinical training tools that have been used in campaigns, for multi-country launches of Nepro Advanced Renal Nutrition Next Generation
- Synthesized content to develop a cohesive brand strategy, created site maps and wireframes, compiled clinical research, and collaborated with colleagues at both domestic sites and international affiliates

## ADDITIONAL EXPERIENCE

*Delegate, UC Berkeley Graduate Assembly (GA)* August 2017-Present

- Serve as one of four delegates from the College of Chemistry to the governing body for all UC Berkeley graduate students and its monthly meetings
- Serve as the graduate member of the Committee on Courses of Instruction (COCI), a UCB Academic Senate committee that meets biweekly
- Served as a member of the 2019 Faculty Mentor Award Committee

*Volunteer, Berkeley High School Bridge Program* September 2017-December 2018

- Serve as an after-school tutor for first-generation college-bound students

*Alumnae Advisory Committee, Pi Beta Phi Sorority, California Beta Chapter* December 2016-Present

- Serve as a member of the alumnae committee that advises the UC Berkeley Pi Beta Phi chapter's undergraduate executive council
- Advise the Vice President of Philanthropy and the Vice President of Administration as necessary on a day-to-day basis to ensure that her responsibilities are being fulfilled

- Colonizing Class Member*, Pi Beta Phi Sorority, Illinois Kappa Chapter March 2013-June 2016
- Policy and Standards Board Member* January-June 2016
- Arbitrated in cases of chapter standards issues and assisted with risk management
- Vice President of Finance* January-December 2015
- Developed and managed an \$80,000+ annual budget, paid chapter bills on a timely basis, maintained accurate records using an online financial system, and prepared and submitted annual tax return for the chapter
- Vice President of Philanthropy* January-December 2014
- Organized 2014 inaugural Arrowfest, a campus philanthropy event that raised more than \$8,000 to benefit youth literacy
- Chair of the Philanthropy Committee* March-December 2013
- Helped coordinate a small spring philanthropy event and presided at committee meetings
- Editor-in-Chief, The Triple Helix Online*, The Triple Helix October 2012-June 2016
- Researched, wrote, and edited quarterly online articles on contemporary medical and technological issues such as social media and organ donation, 3D printing, living wills, and wearable technology
  - Promoted to managing editor in October 2015—responsible for overseeing all content produced by editors and writers in each cycle
  - Assumed Editor-in-Chief role during Winter 2016
- Treasurer*, Burton-Judson Hall Council School Year 2013-2014
- Elected to manage dormitory finances and help organize quarterly events to promote dorm unity

## HONORS AND AWARDS

*Honorable Mention*, NSF Graduate Research Fellowships Program, 2018

*Recipient*, University of Chicago Materials Research Science & Engineering Center Research Experience for Undergraduates Grant (MRSEC REU), Summer 2015

*Recipient*, Jeff Metcalf Fellowship Grant for Internships (Collaborative Learning in Chemistry Team Leader), School Years 2013-15

## OTHER SKILLS

- Experienced in Windows, Mac, and Linux operating systems and software
- Proficient in C++, Python, Java, and Mathematica
- Experience with Scheme and SQL
- Native speaker of English, proficient in French, intermediate knowledge of Czech