

Katherine J. Oosterbaan

kjoosterbaan@gmail.com

Berkeley, CA

EDUCATION

The University of California, Berkeley, Berkeley, CA

PhD Candidate in Theoretical Chemistry

August 2016-Present

Designated Emphasis, Computational and Data Science and Engineering

Advisor: Martin Head-Gordon

The University of Chicago, Chicago, IL

B.S. in Chemistry with Honors

2012-2016

Minor in Slavic Languages and Literatures – Czech

Honors Thesis: "Two Methods for Potential Use in Water Purification"

Berkeley Coursework: CHEM 220A Thermodynamics and Statistical Mechanics; CHEM 221A-221B Advanced Quantum Mechanics 1-2; COMPSCI C267 Applications of Parallel Computers; CS61A Structure and Interpretation of Computer Programs; CS61B Data Structures; NE C285 Nuclear Security; STAT 243 Introduction to Statistical Computing

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

“Generalized single excitation configuration interaction: an investigation into the impact of the inclusion of non-orthogonality on the calculation of core-excited states,” K. J. Oosterbaan, A. F. White, D. Hait, and M. Head-Gordon. *Phys. Chem. Chem. Phys.* **22**, 8182 (2020).

“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

Data Science Education Program Fellow, UC Berkeley D-Lab

January 2020-Present

- Guide undergraduates developing data science teaching materials intended to introduce a data science element to a broad range of Berkeley courses
- Meet with undergraduate developer teams weekly, conduct code reviews and debugging, develop code when needed, and give feedback on drafts
- Advise undergraduates on mentorship and leadership as they oversee their own developer teams

Member, Science and Arts Academy (SAA) Board of Trustees 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
- Received Outstanding GSI from the UC Berkeley Graduate Division
- 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

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
- Former advisor to the Vice Presidents of Philanthropy and Administration

Finance/Housing Advisor

December 2019-Present

- Maintain financial stewardship of the chapter and collaborate with the Chapter House Corporation to run the chapter facility
- Advise and mentor the Vice President of Finance and Housing, Director of Housing, and Director of Member Finances

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
- Elected as a graduate delegate for the 2019-2020 academic year to UC Berkeley's Graduate Council, a UCB Academic Senate committee that meets once a month
- 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 and the 2020 Carol D. Soc Award Committee

Volunteer, Berkeley High School Bridge Program

September 2017-December 2018

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

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

Chemistry Instructional Achievement Award, UC Berkeley Department of Chemistry, 2020

Outstanding GSI Award (Chem 120A), UC Berkeley Graduate Division, 2020

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, R, and Mathematica
- Experience with Scheme and SQL
- Native speaker of English, proficient in French, basic knowledge of Czech