

Jacob Z. Williams

Quantum chemistry and quantum computation

Information

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Skills

Quantum chemistry

- Quantum ESPRESSO ● ● ●
- wannier90 ● ● ●
- Gaussian ● ● ●

Programming

- Fortran ● ● ●
- R ● ● ●
- Bash ● ● ●
- Python ● ● ●
- C++ ● ● ●

Tutoring

- CRLA certification ● ● ●

Languages

- English ● ● ●
- German ● ● ●

Affiliations

- ACS (2016–)
- AMS (2018–)
- APS (2020–)

About

- Piano: early intermediate
- Go: 8k (OGS)
- Erdős number: 5

Education

Ph.D. Chemistry

Localized orbital scaling correction for materials and interfaces
Duke University | 2019–ongoing

B.S. Chemistry

ACS approved degree
University of Wyoming | 2014–2019

- Minor: University Honors Program

B.S. Mathematics

Concentration: Applied mathematics
University of Wyoming | 2014–2019

- Minor: Computer Science

B.S. Statistics

On the economics of player-vs.-player ship combat in EVE Online
University of Wyoming | 2014–2019

Preprints and publications

- Williams, J. Z.; Yang, W. Localized orbital scaling with linear-response curvaturer (in preparation).
- Mahler, A.; Williams, J. Z.; Su, N. Q.; Yang, W. Localized orbital scaling correction for periodic systems. *Phys. Rev. B* **106**, 035147 (2022).
- Mahler, A.; Williams, J. Z.; Su, N. Q.; Yang, W. Wannier Functions Dually Localized in Space and Energy. *arXiv:2201.07751* (2022).
- Wright, A. M., et al. Experimental and Computational Investigation of the Aerobic Oxidation of a Late Transition Metal-Hydride. *J. Am. Chem. Soc.* **141**, 10830 (2019).
- Morrow, T. J.; Christman, W. E.; Williams, J. Z.; Navamoney, A.; Hulley, E. B. Ligand dynamics and protonation preferences of Rh and Ir complexes bearing an almost, but not quite, pendent base. *Dalton Trans.* **47**, 2670 (2018).

Presentations

5. Williams, J.; Yang, W. Curvature and unit-cell periodicity in the localized orbital scaling correction (American Physical Society; Las Vegas, 2023).
4. Williams, J.; Mahler, A.; Yang, W. Localized orbital scaling correction with screened Coulomb interaction (American Chemical Society; Atlanta, 2021).
3. Williams, J. Z.; Shader, B. L. Maximum efficiency, minimum effort: Fastest-mixing Markov chain on (m, n) -star graphs (Joint Mathematics Meetings; Baltimore, 2019).
2. Williams, J.; Merz, D.; Dima, R. I. Allosteric mechanism of peptide release in the molecular chaperone Hsp70 (American Chemical Society; New Orleans, 2018).
1. Williams, J.; Wright, A. M.; Goldberg, K. I.; Cundari, T. R. Oxidation of an iridium hydride pincer catalyst by O₂: A DFT study (American Chemical Society; San Francisco, 2017).

Research experience

Graduate research assistant

Advisor: Weitao Yang
Duke University | 2020–

Extension of the localized orbital scaling correction (LOSC) method to periodic boundary conditions.

- Investigated properties of dually localized Wannier functions (DLWFs);
- Implemented and characterized phenomenological Coulomb and beyond-RPA linear-response screening between DLWFs, necessary for treatment of solids;
- Refactored the FORTRAN prototype of LOSC from the `PostProc` module of Quantum ESPRESSO version 6.3 to a standalone module in a fork of the development version;
- Applications to include heterogeneous catalysis and solar cell design.

Wyoming Research Scholars Program

Advisor: Bryan Shader
University of Wyoming Department of Mathematics | 2018–2019

Properties of the fastest-mixing Markov chain for a family of highly symmetric ‘star-like’ graphs.

- Leveraged computational techniques from convex and semidefinite optimization;
- Computationally simplified problem by analytic techniques and exploitation of symmetries.

Research Experience for Undergraduates

Advisor: Ruxandra Dima
University of Cincinnati Department of Chemistry | 2017

Simulated laser optical tweezer experiments probing the unfolding dynamics of molecular chaperone Hsp70.

- Used in-house, GPU-accelerated, coarse-grained molecular dynamics code;
- Analyzed >100 GB of data with Python and Bash.

Research Experience for Undergraduates

Advisor: Tom Cundari
University of North Texas Department of Chemistry | 2016

Reaction energetics and mechanism of oxygen insertion into an iridium hydride pincer catalyst by DFT.

- Collaborated with experimentalists in NSF CCI: Center for Enabling New Technologies through Catalysis;

- Combined real and computational experiments to determine mechanistic pathway.

Undergraduate research

Advisor: Elliott Hulley

University of Wyoming Department of Chemistry | 2015–2017

DFT calculations of structure, energetics, and dynamics on rhodium and iridium complexes.

- Performed computational experiments with Gaussian;
- Early on, aided in synthetic experiments.

Applications chemist intern

Snowy Range Instruments | 2015

Developed a multivariate method to classify herbal products by Raman spectroscopy.

- Obtained Raman spectra of 20 commercial and whole-plant herbs supplied by collaborator;
- Classified spectra by principal components analysis.

Teaching experience

SPIRE tutor

Duke University | 2020

Individual tutoring for students in STEM Pathways for Inclusion, Readiness, and Excellence.

- General (spring) and physical (fall) chemistry.

Advanced chemistry TA

Duke University | 2019–2020

Analytical chemistry (fall 2019), physical chemistry (spring 2020).

- Validated data and instructed use of advanced instrumental techniques (HPLC, CV, CC, AA, AE);
- Facilitated discussion of data analysis and computational tools (MATLAB, Spartan);
- Collaboratively graded lab reports and exams.

General chemistry TA

University of Wyoming | 2018–2019

Laboratory and discussion sections.

- Upheld safety standards, enforced policy, and administered labs independently;
- Facilitated weekly discussions and quizzes and held group and individual study sessions;
- Graded lab reports, quizzes, and exams.

Tutor

University of Wyoming | 2018–2019

Experienced with group and individual, appointment and walk-in tutoring.

- Tutored mathematics (algebra, trigonometry, calculus, differential equations), statistics, general and organic chemistry;
- Attained CRLA level II: Advanced Certified Tutor.

Service

Triangle Molecular Simulation Society

Duke University | 2021–2022

- Co-organized first annual TriMoIS symposium
- Website manager for 2022

Graduate Christian Fellowship

Duke University | 2021–

- 2022 *et religio* dinner dialogue on science and faith
- Student leader for biweekly science and faith discussion
- Coordinator for weekly small group for graduate students and postdocs

Graduate Chemistry Council

Duke University | 2020–

Vice President, 2022–2023; Treasurer, 2020–2022.

- Co-organized departmental research symposium in 2021 and 2022
- Recruitment host for incoming students, 2020–2022

American Chemical Society Student Affiliates

University of Wyoming | 2017–2019

- Served as President (2017), Secretary (2016, 2018);
- Organized and led chemical demonstrations for local schoolchildren (2017–2018);
- With local ACS section, hosted National Chemistry Week Program-in-a-Box webinar (2017);
- Organized New Belgium brewery microbiological and chemical laboratory tour (2018).

Awards

Charles Bradsher Memorial Fellowship

Duke University | Fall 2022

University Honors Program

University of Wyoming | 2014–2019

Clifford C. Hach Memorial Scholarship

Academic merit in chemistry

University of Wyoming | 2014–2019

Dr. J. Ray Hanna Scholarship

Academic merit in mathematics

University of Wyoming | 2018–2019

Trustees' Scholars Award

Full-tuition award for academic merit

University of Wyoming | 2014–2017

Owen Asplund Memorial Prize

Academic excellence in chemistry

University of Wyoming | 2016

President's and Dean's List

3.5 GPA (Spring 2015), 4.0 GPA (other semesters)

University of Wyoming | 2014–2019