Paige E. Bowling

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EDUCATION

The Ohio State University *(Columbus, Ohio)* ……*AU18 to AU24*
M.S. Biophysics (Candidacy)
Ph.D. Candidate Biophysics

Colorado School of Mines (*Golden, Colorado)* …… *AU13 to SP18*
B.S. Chemistry with a Biochemistry Specialty
B.S. Chemical & Biochemical Engineering

RESEARCH

University of Michigan

Post-Doctoral Science Advisor: Dr. Charles L. Brooks III……...SP25 to Present
Post-Doctoral AI Advisor: Dr. Ambuj Tewari……..AU25 to Present
Eric and Wendy Schmidt AI in Science Postdoctoral Research Fellow 2025 - Machine learning to improve landscape flattening for Multisite λ-Dynamics (MSλD).

Focus on advancing methods to explore chemical space efficiently using MSλD (GitHub Repository). Conceptualize and investigate innovative strategies, including integration of machine learning, to enhance the accuracy and speed of identifying potential therapeutics.

The Ohio State University

Doctoral Advisor: Dr. John Herbert ……SP19 to AU24
Thesis: "Quantum Mechanical Approaches for Large Protein Systems: Fragmentation, Confining Potentials, and Anisotropic Solvation"

Applied and extended existing computational quantum chemistry methods to large protein systems. Contributed to the creation, development, and maintenance of an open-source software package for molecular fragmentation (GitLab Repository). Developed protocols to improve the accuracy of predicting protein energetics towards the complete basis set limit.

Colorado School of Mines

Undergraduate Advisor: Dr. Shubham Vyas…….SP17 to SP18
Undergraduate Advisor: Dr. Brian Trewyn……....AU13 to AU16

PAPERS

[In Preparation] **P. E. Bowling,** D. R. Broderick, J. M. Herbert. "Application of Energy-Based Screening to Fragmentation Predict the Binding Energies of Metalloenzymes."

[Submitted] **P. E. Bowling,** J. Z. Vilseck, C. L. Brooks III. "Accelerated Combinatorial Drug Design for Human Immunodeficiency Virus Resistance Through Seeded Multisite λ-Dynamics."

[Submitted] D. R. Broderick, **P. E. Bowling,** C. Brandt, S. Childress, J. Higley, J. Shockey, H. Dickerson, S. S. Ahmed, J. M. Herbert. "Fragme∩t: An open-source framework for multiscale quantum chemistry based on molecular fragmentation." ChemRxiv doi:10.26434/chemrxiv-2025-1k4k6

P. E. Bowling, M. Gray, S. K. Paul, and J. M. Herbert. "Testing Heterogeneous Polarizable Continuum Models Against Exact Poisson Boundary Conditions." *JCTC* **2025**, 21, 4, 1722–1738.

P. E. Bowling, D. R. Broderick, and J. M. Herbert. "Quick-and-Easy Validation of Protein-Ligand Binding Models Using Fragment-Based Semi-Empirical Quantum Chemistry." *JCIM* **2025**, 65, 2, 937–949.

P. E. Bowling, D. R. Broderick, and J. M. Herbert. "Convergent Protocols for Protein-Ligand Interaction Energies Using Fragment-Based Quantum Chemistry." *JCTC* **2025**, 21, 2, 951–966.

M. Gray, **P. E. Bowling,** and J. M. Herbert. "Comment on: Benchmarking Basis Sets for Density Functional Theory Thermochemistry Calculations: Why Unpolarized Basis Sets and the Polarized 6-311G Family Should Be Avoided" *J. Phys. Chem. A.* **2024**, 128, 36, 7739–7745.

P. E. Bowling, S. Dasgupta, and J. M. Herbert. "Eliminating imaginary frequencies in quantum-chemical cluster models of enzyme active sites." *JCIM.* **2024** 64, 3912–3922.

P. E. Bowling, D. R. Broderick, and J. M. Herbert. "Fragment-based calculations of enzymatic thermochemistry require dielectric boundary conditions." *JPC Let.* **2023** 14, 3826–3834.

M. Gray, **P. E. Bowling,** and J. M. Herbert. "Counterpoise Correction in Density Functional Theory." *JCTC* **2022**, 18, 11, 6742–6756.

PRESENTATIONS

- Midwest Theoretical Chemistry Conference - Wayne State University, Detroit, MI. In person, May 2025.
- National Spring ACS Conference - New Orleans, LA. Quantum Mechanics, Division of Computers in Chemistry. In-person, March 2024.
- National Spring ACS Conference - New Orleans, LA. Women Make COMP, Division of Computers in Chemistry. In-person, March 2024.
- Midwest Theoretical Chemistry Conference - Purdue University, West Lafayette, IN. Biophysics and Statistical Mechanics. In-person presentation, June 2023.
- Interdisciplinary Graduate Program Symposium - Ohio State University, OH. Plenary Speaker, May 2023.
- National Spring ACS Conference - Indianapolis, IL. QM/QM and Embedding Models, Comp Division. In-person, March 2023.
- Biophysics Program Seminar - Ohio State University, OH. Hybrid presentation, September 2022.
- National Spring ACS Conference - San Diego, CA. New Developments in Hybrid QM/MM, QM/MM, and Fragmentation Methods Symposium, Physical Division. In-person, March 2022.

HONORS & AWARDS

OSU Interdisciplinary Graduate Program Symposium…….....Outstanding Poster Presentation 2024

American Chemical Society .....Graduate Student and Postdoctoral Scholars Recognition 2023

The award is presented to graduate students and postdoctoral scholars who've demonstrated exemplary achievements in any of the three categories: leadership in mentoring, the promotion of Diversity, Equity, Inclusion, and Respect (DEIR), or the promotion of research safety. Received the award for mentorship.

OSU Chemistry Department .....John S. Swenton Award for Outstanding Teaching 2023

Nominated by two faculty members whom I had taught with. The award stated: "She has demonstrated a strong level of dedication to teaching and learning and [has] gone above and beyond to help her students understand difficult and abstract concepts using advanced math. The instructors who have supervised her as a GTA describe Paige as one of the most efficient, reliable, and thorough GTAs they have ever worked with."

Society of Women Engineers .....Outstanding Collegiate Member (National Award) 2017

Bestowed upon SWE collegiate members who have made an outstanding contribution to SWE, the engineering community, and their campus.

Colorado School of Mines .....E-Days Engineer 2016

An annual award designed to recognize outstanding seniors for their hard work and dedication to the Mines community.

SELECTED PROJECTS & SOFTWARE

Oxford Loss Landscapes……[GitHib Repository]

Contributor to "loss landscapes for explainable AI" project, which is a Python library for visualizing and analyzing neural network loss landscapes. Developed as part of the 2025 Research Software Engineering workshop at Oxford University.

MENTORSHIP

UROP Lead Investigator, University of Michigan……*AU25 to Present*

Mentored Undergraduate Research Opportunity Program (UROP) students in computational research projects utilizing MSλD in CHARMM molecular dynamics software. Provided hands-on instruction in setting up and running molecular dynamics simulations, including use of HPC resources, Linux command-line operations, basic Bash scripting, and Slurm workload management.

REU Graduate Mentor, The Ohio State University……..*SU20, SU 23, SU24*

Supervised and mentored undergraduate students participating in a National Science Foundation Research Experiences for Undergraduates (REU) program focused on the development of a novel molecular fragmentation quantum chemistry software package. Taught core computational research skills, including code development, writing unit tests, and debugging.

LEADERSHIP, SERVICE, & PROFESSIONAL MEMBERSHIP

University of Michigan Postdoctoral Association (UMPDA).....*SP25 to Present*

Serve as Public Relations Chair as of Summer 2025; responsible for organizing and curating outreach and website materials, as well as maintenance of the UMPDA mission.

American Chemical Society (ACS) .....*SP22 to Present*

Active member and presenter in COMP and PHYS divisions. COMP session chair SP22, SP23, SP24, & AU24.

Biophysics Student Organization (BSO).....*AU18 to AU24*

Positions Held: President, Treasurer, Secretary, & Second-Year Representative

Served in many roles with various responsibilities, including serving as the Graduate Council Student representative, maintaining the financial health of the BSO and applying for funding, planning and hosting student events, and participating in and leading program recruitment.

Joint Diversity Team (JDT).....*SP20 to AU24*

Positions Held: Lab Coordinator, Member of LGBTQIA+ Committee

Serve as the liaison between the Herbert group and the Chemistry department JDT. JDT's goal is to promote awareness of racial, gender identity, sexuality, and student-parental status issues.

OSU Rock Climbing Team.....*AU18 to SP24*

Positions Held: President & Coach, Treasurer

Founded the club in the fall of 2018 after coming to OSU, and have been personally responsible for planning and coaching team practices, recruitment, and maintaining strong relationships with local gyms and outdoor groups.

TEACHING EXPERIENCE

The Ohio State University

ACS Bridge Program Tutor……..*AU22 to SP24*

Tutored ACS Bridge Program students in graduate-level physical chemistry, utilizing equitable and inclusive teaching methods to support diverse learners.

Physical Biochemistry II (BIOCHEM5722) ……..SP23

Teaching assistant for undergraduate-level course for upperclassmen. Serves as an introduction to quantum chemistry for chemistry (B.A.) and biochemistry majors. This course covers the

experiments that led to the development of quantum theory as well as fundamental concepts, equations, and problems in quantum mechanics and spectroscopy.

Physical Chemistry (CHEM4300) ……...AU19, AU20, SP20, AU22
Teaching assistant for undergraduate-level course for upperclassmen. Serves as an introduction to quantum chemistry for chemistry (B.S.) and chemical engineering majors. Students are taught quantum mechanics and develop first-principles framework for understanding molecules and chemical bonding.

Introduction to Electronic Structure Theory (CHEM6540) ……..AU21
Teaching assistant for graduate-level course for first-year physical chemistry students. Students learn fundamental theory behind computational quantum chemistry techniques and apply them. Students develop basic proficiency with Linux OS and using high-performance computing environments.

Statistical Thermodynamics (CHEM4310) ……....SP20
Teaching assistant for undergraduate-level course for upperclassmen serves as an introduction to thermodynamics. Students derive the fundamental concepts needed to understand an ensemble under different conditions.

Colorado School of Mines

Principles of Chemistry I (CHGN121) ……..AU17
Served as a lab teaching assistant, worked with 24 students of varying proficiencies to transition them from high school to a collegiate lab setting to applied chemistry, and teach them introductory lab and safety procedures.

SKILLS DEVELOPMENT

- “Research Software Engineering Training Programme” - Schmidt AI and University of Oxford. **September 2025.**
- “Knowledge-Guided Machine Learning” - Schmidt AI and Michigan Institute for Data & AI in Society. **August 2025.**
- “Machine Learning for Molecules” - i-CoMSE. **April 2025.**
- “AI in Science and Engineering Symposium,” Michigan Institute for Data & AI in Society. **March 2025.**
- “Promises and Pitfalls of AI for Research and Scholarship Integrity” - Big Ten Academic Alliance’s Responsible Conduct of Research Collaborative. **November 2024**.
- "Python Scripting for Molecular Docking" - RCSB Protein Data Bank. **July 2024.**
- “Big Data & Machine Learning” - PSC ACCESS HPC. **March 2023.**
- “Methods for Advanced Sampling” - i-CoMSE. **March 2023.**
- “An Introduction to Evidence-Based STEM Undergraduate Teaching” - The CIRTL Network. **Nov 2021.**