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 Advisor: Dr. Charles L. Brooks III…….SP25 to Present
Eric and Wendy Schmidt AI in Science Postdoctoral Research Fellow 2025 - Reinforcement learning to improve landscape flattening for Multisite Lambda Dynamics (MSLD).

Focus on advancing methods to explore chemical space efficiently using MSLD. 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 (written in Python for fragmentation) for molecular fragmentation. 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."

[In Preparation] D. R. Broderick, **P. E. Bowling,** H. Dickerson, J. Higley, J. Shockey, and J. M. Herbert. "Fragme∩t: An Extensible Framework for Fragmentation."

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 for. 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.

LEADERSHIP & PROFESSIONAL MEMBERSHIP

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

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.

WORKSHOP PARTICIPATION

- “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.**

SKILLS

QM & MM Packages: QChem, Orca, xTB, Molecular Dynamics (CHARMM, AMBER, GROMACS), AutoDock Vina

Coding Languages: Python, C++, C, Java, Bash scripting

Data Analysis & Visualization: R, Adobe Illustrator, Matlab, Mathematica, Visual Tool Kit (VTK)