Devin Mulvey

Curriculum Vitae

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Note: Boldface text throughout the document is a hyperlink. For example, this is my **Google Scholar.**

Education

2018-2023 Ph.D. Chemistry (Physical Chemistry)
- University of Pittsburgh
- Advisor: **Kenneth Jordan**
- GPA: 3.75
- Thesis:**"Bridging the Gap: Demonstrating the Connection Between Non-Valence Correlation-Bound Anions and Image Potential States Using a One-Electron Model"**

2015-2018 B.S. Chemistry and B.A. Mass Communications (Journalism),
- **Bloomsburg University**
- GPA: 3.62

Academic Positions Held

Fall 2024 - Present Postdoctoral Researcher and Lecturer – St. Bonaventure University
- Advisor: **Scott Simpson**
- Job duties include:
  - Teaching
  - Research
  - Course development
  - Grant writing
  - Outreach

Summer 2018 - Fall 2023 Research and Teaching Assistant – University of Pittsburgh
- Job duties included:
  - Recitation Lectures
  - Research
  - Undergraduate and high school research mentorship
  - Grant writing

Courses Taught

St. Bonaventure University (Instructor of Record)
- CHEM-091 – Problem Solving in Chemistry
- CHEM-101 – General Chemistry I Lecture
- CHML-101 – General Chemistry I Lab
- CHEM-102 – General Chemistry II Lecture
- CHML-102 – General Chemistry II Lab
- CHML-402 – Physical Chemistry II Lab (Anticipated for SP 2026)
- CHEM-498 – Undergraduate Research (Anticipated for SP 2026)

University of Pittsburgh (TA)
- CHEM-0970 – General Chemistry for Engineers II
- CHEM-0120 – General Chemistry II
- CHEM-0110 – General Chemistry I

Technical Skills

Certifications: OREC Sections 1 and 6 for Human Participants, SEHSA/RCRA Chemical Waste Handling Certified

Programming: Python, C++/C, Bash (Linux, Unix CLI), LaTeX

Software: LOBSTER, VASP, Psi4, Orient, CamCASP, Molpro, ORCA, CFOUR, Gaussian, PySCF, Spartan, VMD, Avogadro, MS Office, LibreOffice

LMS Moodle

OS Windows, Linux, macOS

Research

2024-Present My post doctoral work consists of both scientific and educational research.

- Scientific research: I investigate the molecular corking effect, where ligands like N-heterocyclic carbenes (NHCs) selectively and reversibly bind to catalytic atoms in single-atom alloys (SAAs), using van der Waals-corrected DFT and localized orbitals from plane-wave basis sets.
- Educational research: I study the integration of generative AI into chemistry curricula, focusing on AI-assisted lab and lecture assignments that teach prompt engineering, data analysis, and safe, critical use of third-party tools like OpenAI.

2019-2023 The core of my doctoral research was developing approximate, but quantitatively accurate models to describe the non-valence correlation-bound (NVCB) anions of finite analogues of graphene, referred to as polycylic aromatic hydrocarbons (PAHs) and graphene nanoflakes. Accurately modeling the non-covalent interactions stabilizing these anions is a challenge in and of itself, but the culmination of my research enabled us to draw a connection between the NVCB anions of these finite hydrocarbons and the analogous loosely-bound anionic states of graphene, referred to as image potential states.

2020-2022 I collaborated with members of the Jordan group and researchers from Pitt's Schools of Computing and Information (Tang group) and Electrical and Computer Engineering (Yang group) to develop Q-GPU, a framework integrated into **Qiskit** for efficiently simulating quantum circuits on classical hardware. Q-GPU leverages both CPU and GPU resources to simulate systems with tens of qubits, providing a scalable alternative to physical quantum computers.

2016-2018 **Used DFT and the Born-Haber cycle** to assess the radical scavenging capabilities of fullerenols $\mathrm{C_{60}(OH)_n}$ $(\mathrm{n} = 1, 2, 3, \dots)$. Began developing graph representations to identify and categorize the symmetry and electrostatics of hydrogen bonding networks on the surface of fullerenols as a predictor of antioxidant activity.

Publications

- D. M. Mulvey and S. M. Simpson,"Characterizing σ donation and π backbonding for simple, representative molecular "corks" on Cu/Pd SAA Surfaces", 2025 [In-Preparation].
- D. M. Mulvey and S. M. Simpson,"Exploring Generative AI Application in General Chemistry: A Lab-Based Study of AI Assisted Analysis and Critical Evaluation of AI Generated Outputs", 2025 [In-Preparation].
- D. M. Mulvey, K. D. Jordan, M. J. Rutter, and A. J. Misquitta,"A Practical Electrostatic Model for Hexagonal Polycyclic Aromatic Hydrocarbons and Carbon Nanoflakes: Implications for Graphene", 2025 [In-Preparation].
- S. M. Simpson and D. M. Mulvey,"Tools for Understanding Molecular Orbitals Interactions of Molecules on Surfaces - Density Functional Theory Calculations of $\mathrm{H_2}$ Adsorbed on Cu(111) and Pd/Cu(111)", Ind. Eng. Chem. Res., (2025) [**Submitted**].
- D. M. Mulvey and K. D. Jordan, "Demonstrating the Connection Between Non-valence Correlation-bound Anions and Image Potential States using a One-Electron Model Hamiltonian", J. Phys. Chem. Lett., (2024) **DOI:10.1021/acs.jpclett.4c01308**
- D. M. Mulvey, "Bridging the Gap: Demonstrating the Connection Between Non-Valence Correlation-Bound Anions and Image Potential States Using a One-Electron Model", (2024) **Dissertation Thesis**
- D. M. Mulvey and K. D. Jordan, "Application of a Fluctuating Charge Polarization Model to Large Polyaromatic Hydrocarbons and Graphene Nanoflakes", J. Phys. Chem. Lett. 0, 14 (2023) **DOI: 10.1021/acs.jpclett.3c02013**
- D. M. Mulvey and K. D. Jordan,"Progress Towards a One-Electron Model for the Non-valence Correlation-bound Anions of Polycyclic Aromatic Hydrocarbons", Electron. Struct. 4, 014010 (2022). **DOI:10.1088/2516-1075/ac522a**

- Y. Zhao, Y. Guo, Y. Yao, A. Dumi, D. M. Mulvey, S. Upadhyay, Y. Zhang, K. D. Jordan, J. Yang, and X. Tang, "Q-GPU: A Recipe of Optimizations for Quantum Circuit Simulation Using GPUs", International Symposium on High-Performance Computer Architecture, (2022), **DOI: 10.1109/HPCA53966.2022.00059**

Financial Support

Spring 2025 - Spring 2026
- **Keenan-Martine Grant**
  - Amount: $ 3978.93
  - Title: Enhancing Teaching and Learning in Chemistry Labs via Vernier LabQuest Mini 2 Integration
  - Agency: St. Bonaventure University

Spring 2025 - Spring 2026
- **Keenan-Martine Grant**
  - Amount: $ 3972
  - Title: Fostering GenAI Literacy and Competency as a Tool for Scientific Writing and Data Analysis in Chemistry Courses
  - Agency: St. Bonaventure University

Summer 2018
- **Chair's Scholar Summer Research Fellowship and Excellence Award**
  - Amount: $ 5300
  - Agency: University of Pittsburgh

Scientific Community Engagement

2025
- Presented the following talks at ACS Fall 2025:
  - **Characterizing σ donation and π backbonding in molecular "corks" on copper-palladium single-atom alloy surfaces**
  - **Exploring generative AI application in general chemistry: A lab-based study of prompt engineering, AI assisted analysis, and critical evaluation of AI generated outputs**
- Attended Mercury Consortium 2025 hosted at University of Pittsburgh

2024
- Attended **Mercury Consortium** 2024 hosted at UC Merced.

2022
- Gave an oral presentation at the Tinker Developer Workshop.
- Gave an oral presentation at the TSRC summer school, **"Many-Body Interactions: From Quantum Mechanics to Force Fields"**.

2021
- Gave an oral presentation at the **Advanced Force Fields symposium** at the Fall National ACS meeting.
- Gave an oral presentation at the **Real Space Methods for the Electronic Structure Problem: Dynamics and Applications** Session at the March National APS meeting.

2020 Attended the virtual TSRC summer school, **"Many-Body Interactions: From Quantum Mechanics to Force Fields"**.

Outreach: Past and Present

High School Summer Research Mentorship (2025) Developed and implemented a high school research project providing a broad introduction to computational and theoretical chemistry. The student built a Raspberry Pi 5 to explore computing hardware, then used it to access a university cluster via SSH. They ran quantum chemical calculations to model the hydrogen atom transfer (HAT) mechanism of ascorbate anion as a free radical scavenger, analyzed the results, and presented their findings, gaining experience across the full computational chemistry pipeline.

ICE-T (2018) Worked with high school students to develop novel solutions for microbial fuel cells ("living batteries"), providing guidance on lab procedures, literature review, hypothesis development, and research presentations. Taught students the fundamentals of microbial fuel cell theory, how to make and interpret performance measurements, and led Python coding exercises covering programming basics, data collection, analysis, and plotting.

Research Mentoring (2018-2021) As a graduate student I worked with high school students on computational projects within the atmospheric chemistry and biochemistry domains. Provided assistance in literature review, hypothesis development, preparation and running of simulations, and preparation of papers and oral presentations summarizing their research.