Malachi Kent

Curriculum Vitae
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RESEARCH INTERESTS

Theory development and computational implementation of high-accuracy electronic structure methods, specifically cluster perturbation theory, for predicting molecular properties such as ionization potentials, electron binding energies, and response properties with specific interested in making accurate many-body methods more efficient. This includes automating the derivation of their underlying equations, turning theory into reliable, high-performance code, and testing that code rigorously. Broader interests include high-performance scientific computing and applications of quantum computing in chemical simulation.

EDUCATION

Ph.D., Chemistry (Quantum/Computational Focus) | Auburn University — Expected May 2027

Dissertation Focus: Cluster perturbation theory for electron binding energies and molecular response properties

Relevant Coursework: Quantum and Statistical Mechanics, Computational Methods, Molecular Spectroscopy, Machine Learning, Deep Learning

B.S., Biochemistry, Minor in Mathematics | Georgia Southern University (Honors College) — May 2021

IBM Basics of Quantum Information | Asynchronous course — In Progress

RESEARCH EXPERIENCE

Graduate Researcher | Auburn University, Department of Chemistry and Biochemistry — Aug 2023 – Present

- **Many-Body Method Development:** Develop and implement cluster perturbation methods, built on the coupled cluster framework, for ionization potentials, electron binding energies, and molecular response properties.
- **Implementation:** Implement new methods in a standalone code interfaced with Psi4, assessing accuracy against computational cost relative to established coupled cluster methods.
- **Symbolic Automation:** Creating programs that automate the derivation of second-quantized commutator expressions and generate implementation code directly, reducing manual error in complex many-body equations.
- **Testing Architecture:** Developing a modern testing architecture to support maintenance of current and new code repositories.
- **Collaboration:** Collaborate with faculty and peers on novel computational algorithms and prepare results for publications and presentations.

Research Student Intern | Oak Ridge National Laboratory, Computing and Computational Sciences — May 2025 – Aug 2025

- **Tensor Software:** Developed a Python Interface for a high performance parallel Fortran tensor library (ScaTeLib) using iso_c_binding, ctypes, and NumPy to enable large-scale tensor computations on HPC systems.
- **Parallel Computing:** Resolved MPI synchronization issues, including deadlocks and race conditions, in a mixed-language parallel environment.
- **Software Design:** Engineered a dynamic configuration system that automatically aligns Python's ctypes with compiled Fortran data types, ensuring cross-platform compatibility.
- **Deployment:** Independently deployed and validated the interface on a SLURM-managed HPC cluster.

Undergraduate Research Assistant | Georgia Southern University, Chemistry and Mechanical Engineering — Jan 2019 – May 2021

- Conducted materials characterization and organic synthesis of functionalized nanoclays in an interdisciplinary team, contributing to nanocomposites with improved fracture toughness (published, SN Appl. Sci. 2020).

TECHNICAL SKILLS

- **Many-Body Theory:** Coupled Cluster Theory, Cluster Perturbation Theory, Second Quantization & Commutator Algebra, Molecular Response Theory, Electron Propagator Theory
- **Quantum Computing:** Qiskit (Familiar), Quantum Circuit Construction (Coursework)
- **Scientific Computing:** Python (NumPy, SymPy, Pandas, Matplotlib, Pytest, ctypes), Fortran, C/C++ (Familiar), Psi4, Gaussian (Familiar), VMD
- **HPC:** Linux, HPC Clusters (SLURM), MPI, Parallel Computing, Distributed Tensor Libraries, Git

PRESENTATIONS

- Kent, M. “Cluster Perturbation Theory for Ionization Potentials. Comparison to Electron Propagator Theory.” Southeastern Theoretical Chemistry Association, May 2026

- Kent, M. "Introducing Ionization Potentials in Cluster Perturbation Theory." Poster, Southeastern Theoretical Chemistry Association Conference, May 2025.
- Kent, M. "Introducing Ionization Potentials to Cluster Perturbation Theory." Oral presentation, Sanibel Symposium, February 2025.

PUBLICATIONS

- Dünweber, P. G. I. L., Johansen, M. B., Junker, G. I., Ettenhuber, P., Khan, S. N., **Kent, M.**, Patten, E., Elwasif, W., Bykov, D., Mikkelsen, K. "ScaTeLib: A Scalable Tensor Library for Massively Parallel Electronic Structure Theory" *J. Chem. Theory Comp*. accepted Oct. 2026

TEACHING AND MENTORING

Graduate Teaching Assistant | Auburn University — Aug 2023 – Present
- Instruct laboratory sections of Fundamentals of Chemistry I and II.

Research Mentor | Auburn University — Aug 2023 – Present
- Mentor undergraduate students in computational chemistry research, fostering independent research skills.

Supplemental Instruction Leader and Laboratory Assistant | Georgia Southern University — Aug 2018 – Dec 2020
- Led study sessions on effective learning strategies and supported students and faculty in chemistry laboratories.

INDUSTRY EXPERIENCE

Quality Control Chemist | Pharmavite, LLC — Mar 2022 – Aug 2023
- Performed analytical testing and instrument validation (ICP-MS, GC, UV-Vis, FTIR); authored SOPs and technical reports under GMP, GLP, and FDA/USP standards.

Quality Laboratory Technician | Baxter International Inc. — Jun 2021 – Mar 2022
- Conducted QA/QC testing and maintained data integrity under FDA, GLP, QSR, and cGMP standards.

LEADERSHIP AND SERVICE

Treasurer | Younger Chemists Committee, Auburn University — Aug 2024 – Present

Recruitment Coordinator | Younger Chemists Committee, Auburn University — Aug 2023 – Aug 2024

STEM Outreach Facilitator | Destination STEM, Auburn University — Oct 2024

Camp Counselor | Summer Science Institute, Auburn University — Jun 2024

HONORS AND AWARDS

COSAM Graduate Student Travel Award, Auburn University — May 2025

College of Undergraduate Research Grant, Georgia Southern University — May 2019

Honors College Graduate, Georgia Southern University — 2017 – 2021

REFERENCES

Filip Pawłowski Ph.D., Assistant Professor | Department of Chemistry and Biochemistry, Auburn University | flp0008@auburn.edu

Dmytro Bykov Ph.D., Group Leader in Computing for Chemistry & Materials | Oak Ridge National Laboratory | bykovd@ornl.gov

[Third reference name, title] | [Institution] | [email]