Austin Ellis

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Summary

Computational chemist specializing in machine learning-accelerated discovery and high-throughput quantum chemistry calculations. Track record of advancing scientific research through innovative methods, collaborative projects, and effective communication of complex concepts. Dedicated to contributing to the scientific community through research, teaching, and outreach initiatives.

Education

- **California State University, Northridge** *2023 - Present*
  Master of Science in Chemistry Los Angeles, U.S.
- **University of Oxford** *2023*
  Certificates in AI and ML; Theory, Practice, Neural Networks, Deep Learning (In-person) Oxfordshire, U.K.
- **University of California, San Diego** *2018 - 2022*
  Bachelor of Science in Pharmacological Chemistry San Diego, U.S.

Awards

- **APS Global Physics Summit DCOMP Travel Award** *2026*
  Denver, CO
- **Second Place, Sigma Xi Research Symposium** *2025*
  Northridge, CA
- **AI4Mat–NeurIPS 2025 Travel Grant** *2025*
  San Diego, CA

Research and Work Experience

- **Graduate Research Assistant - Miao Lab, CSUN** *January 2023 - Present*
  - Perform high-throughput calculations using developed and optimized python code for efficient automation and results analysis
  - Fine-tune foundational ML models for efficient materials screening to reduce computational expense, validate with quantum chemistry calculations
  - Prepare weekly presentations for group meetings on topics in machine learning, quantum chemistry, materials science, and specific research updates
  - Independently manage and execute research projects through full project lifecycle from method development and high-throughput calculation to manuscript preparation
  - Created figures and summaries for DoD and NSF reports and presentations
- **HPC Cluster Manager - Miao Lab, CSUN** *August 2023 - Present*
  - Administer, monitor, and optimize the High-Performance Computing (HPC) environment, ensuring consistent uptime and efficient job scheduling
  - Improved cluster efficiency 48x by allowing oversubscription of nodes and optimizing cores per submitted jobs
  - Administered 2 GPU cluster nodes (4× A100s each), performing driver/kernel upgrades, remote power-cycle recovery, and proactive troubleshooting to ensure maximum uptime and reliability for large-scale HPC/ML training
  - Prepared HPC accounts and environments for CSUN faculty and students to perform quantum chemistry calculations for their research/classes

Publications

[4] **Pressure-induced Redox Reversal of Iron and the Distribution of Elements in Deep Earth**
X. Wang, X. Feng, J. Li, Y. Lv, **A. Ellis**, S. Scott, A. Pandit, D. Khodagholian, R. J. Hemley, M. G. Jackson, F. J. Spera, S. A. T. Redfern, M. Miao *Proceedings of the National Academy of Sciences*. **2025**, 122, e2414911122. DOI: 10.1073/pnas.2414911122

[3] **Batch Discovery of Complex Metal Superhydrides via an Effective Machine Learning Method Structured by Chemical Template Concept**
Y. Sun, **A. Ellis**, X. Chen, M. Miao *Journal of the American Chemical Society*. **2025**, 147(44), 40407–40419. DOI: 10.1021/jacs.5c11731

[2] **Unlocking the Origin of High-Temperature Superconductivity in Molecular Hydrides at Moderate Pressures**
W. Zhao, **A. Ellis**, D. Duan, H. Wang, Q. Jiang, M. Du, T. Cui, M. Miao *Advanced Functional Materials*. **2025**, 35, 2415910. DOI: 10.1002/adfm.202415910

[1] **Constructing Tunable Electrides on Monolayer Transition Metal Dichalcogenides**
Y. Sun, **A. Ellis**, S. Diaz, Wei Li, and M. Miao *The Journal of Physical Chemistry Letters*, **2024** 15(23), 6174-6182. DOI: 10.1021/acs.jpclett.4c01263

Conference and Workshop Publications

[2] **Symmetry-Aware Prediction of Electron Localization Functions from Superposed Atomic Densities**
A. Ellis, M. Miao *NeurIPS 2025 Workshop (AI4Mat)*. Poster, published on OpenReview September 20, 2025.

[1] **An Effective Machine Learning Frame for Materials Discovery Structured by a Chemical Concept**
Y. Sun, **A. Ellis**, X. Chen, M. Miao *NeurIPS 2025 Workshop (AI4Mat)*. Poster, published on OpenReview November 5, 2025.

Manuscripts in Draft

[3] **Insulator to Metal Transition of Molecular Hydrogen Under Pressure**
A. Ellis, S. Scott, A. Pandit, M. Miao. *Anticipated Submission by April 2026*

[2] **Elucidation of α-Manganese Structure Under Increased Pressure**
A. Pandit, **A. Ellis**, S. Scott, M. Miao *Anticipated Submission by April 2026*

[1] **Monolayer to Bulk Transition of Transition Metals**
A. Ellis, Y. Sun, M. Miao. *Anticipated Submission by April 2026*

Presentations

- **A. Ellis**, Y. Sun, X. Chen, and M. Miao: *An Effective Machine Learning Frame for Materials Discovery Structured by a Chemical Concept*. Talk given at the 2026 CSUN Research and Creative Works Symposium (CSUNposium), Northridge, California, April 2026. (Scheduled)
- **A. Ellis** and M. Miao: *Symmetry Aware Prediction of Electron Localization Functions from Superposed Atomic Densities*. Talk given at the 2026 American Physical Society March Meeting (APS), Denver, Colorado, March 2026. (Scheduled)
- **A. Ellis** and M. Miao: *Symmetry Aware Prediction of Electron Localization Functions from Superposed Atomic Densities*. Poster presentation at the 2026 Gordon Research Conference on Enabling Multifunctionality through AI Informed Material Discovery and System Design, Ventura, California, January 2026.
- **A. Ellis** and M. Miao: *Symmetry Aware Prediction of Electron Localization Functions from Superposed Atomic Densities*. Talk given at the 2025 CSUN Sigma Xi Research Symposium, Northridge, California, December 2025.
- **A. Ellis**, Y. Sun, X. Chen, and M. Miao: *An Effective Machine Learning Frame for Materials Discovery Structured by a Chemical Concept*. Poster presentation at the NeurIPS 2025 AI4Mat Workshop, San Diego, California, December 2025.
- **A. Ellis** and M. Miao: *Symmetry Aware Prediction of Electron Localization Functions from Superposed Atomic Densities*. Poster presentation at the NeurIPS 2025 AI4Mat Workshop, San Diego, California, December 2025.
- **A. Ellis**, S. Scott, A. Pandit, and M. Miao: *Insulator to Metal Transition of Molecular Hydrogen Under Pressure*. Poster presentation at the 2025 CSUN Research and Creative Works Symposium (CSUNposium), Northridge, California, April 2025.
- **A. Ellis**: *Advancements in Machine Learned Interatomic Potentials*. Literature review seminar presented as part of the Master's in Chemistry program, Department of Chemistry and Biochemistry, California State University, Northridge, April 2025.
- **A. Ellis**, Y. Sun, S. Diaz, W. Li, and M. Miao: *Constructing Tunable Electrides on Monolayer Transition Metal Dichalcogenides*. Poster presentation at the 2025 American Physical Society Global Summit (APS), Anaheim, California, March 2025.
- A. Pandit, **A. Ellis**, S. Scott, and M. Miao: *Interactions that Govern the Structure of α-Manganese*. Talk given at the 2025 American Physical Society Global Summit (APS), Anaheim, California, March 2025.
- **A. Ellis**, Y. Sun, S. Diaz, W. Li, and M. Miao: *Constructing Tunable Electrides on Monolayer Transition Metal Dichalcogenides*. Poster presentation at the 2024 CSUN Research and Creative Works Symposium (CSUNposium), Northridge, California, April 2024.
- **A. Ellis**, Y. Sun, S. Diaz, and M. Miao: *Core reactivity of Cs Polyoxides Under Pressure*. Poster presentation at the 2023 UCLA Theoretical Chemistry Conference (TheoChem), Los Angeles, California, October 2023.
- **A. Ellis**, Y. Sun, S. Diaz, and M. Miao: *Applications of OPTIMADE in structure screening within high pressure regimes*. Talk given at the 2023 CECAM Open Databases Integration for Materials Design Workshop, Lausanne, Switzerland, June 2023.
- **A. Ellis**, Y. Sun, S. Diaz, and M. Miao: *Core reactivity of Cs Polyoxides Under Pressure*. Poster presentation at the 2023 CSUN Research and Creative Works Symposium (CSUNposium), Northridge, California, April 2023.

Teaching Experience

- **Physical Chemistry II (CHEM352) - Teaching Assistant** *2024-2025*
  - Lectured two classes of 30 undergraduate students on performing Gaussian calculations in HPC environment
  - Held walk-in hours for students to receive help with calculations and linux environment navigation
- **Computational Molecular and Materials Chemistry (CHEM555L) - Teaching Assistant** *2023*
  - Assisted both undergraduate and graduate students in the class with the completion of final projects, including calculations on Borohydride cages, liquid and solid-state IRs, Raman spec, and solvent effects

Students Mentored

- **Undergraduate Students (Miao Research Group)**
  - S. Scott, Project: Studying hydrogen under pressure with hybrid functionals. Currently pursuing M.S. in Chemistry at CSUN
  - E. Gonzalez, Project: Studying transition of monolayer to bulk transition metals. Currently MCS Associate Quality Control at Amgen
- **Graduate Students (Same CSUN Cohort)**
  - C. Blair (atmospheric chemist), Project: Taught how to use and apply Gaussian (environmental chemistry calculations and the prediction of transition states/reaction kinetics)
  - N. Porcellino (materials chemist), Project: Assisted in calculations of high pressure phases of Ytterbium hydrides. Currently Labaratory Technician at CSL Plasma

Skills

- **Programming Languages:** Python, Bash, C++ (basic; niche CUDA kernel development)
- **Software:** VASP, CALYPSO, AIRSS, Quantum Espresso, Wannier90, Bader, LOBSTER, GULP
- **Database Systems:** MongoDB (limited)
- **Data Science & Machine Learning:** PyTorch, NumPy, Pandas, Tensorflow (limited)
- **Other Tools & Technologies:** LaTeX, Linux/Unix
- **Research Skills:** High-throughput materials calculations, machine-learning for electronic structure, symmetry-aware neural networks, data curation and pre-processing, parallel computing/GPU acceleration, scientific writing

Outreach

- **Chem/Biochem Journal Club - Co-founder September, 2025**: Helped found CSUN's first Chem/Biochem Journal club, curating articles, scheduling presenters, and managing logistics while building participants' paper reading and scientific communication skills through structured discussions, figure analysis, and presentations
- **Chemistry Club Graduate Panel November, 2025**: Invited to speak at Chemistry Club panel to answer undergraduate questions about research in graduate school, application process, and graduate school experience
- **CSUN Research Showcase October, 2025**: Invited by department to present examples of excellent research completed at CSUN for visiting speakers from UCSD, City of Hope, UCI, and USC
- **Chemistry Club "Breaking Science" October, 2025**: Invited to speak at Chemistry Club event to explain and discuss significance of 2025 Nobel Prize in Physics
- **Getting into Research Event September, 2025**: Volunteered with the Office of Undergraduate Research at event focused on assisting undergraduate students get paired with a research lab, delivering research program information and facilitating student-faculty mixer event
- **CSUN Matador Day April, 2025**: Volunteered to present poster on Insulator to Metal Transition of Molecular Hydrogen Under Pressure for incoming high school students, incentivizing interest in research and chemistry program
- **CSUN Science Day April, 2024**: Volunteered to present for local middle school students, showcasing unique chemistry of high pressure systems
- **CSUN Matador Day April, 2024**: Volunteered to present poster on Constructing Tunable Electrides on Monolayer Transition Metal Dichalcogenides for incoming high school students, incentivizing interest in research and chemistry program