Austin Ellis

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Los Angeles, CA, United States

Objective

PhD applicant in theoretical and computational chemistry and materials science with experience in machine learning for electronic-structure methods and high-throughput modeling. Seeking to contribute to cutting-edge research while applying and expanding these skills in a rigorous, collaborative environment.

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

- AI4Mat–NeurIPS 2025 Travel Grant — 2025

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

[4] **Seitz-Invariant Prediction of Electron Localization Functions from Superposed Atomic Densities via a 3D-Convolutional Network**
A. Ellis, M. Miao. *Anticipated Submission April 2026*

[3] **Insulator to Metal Transition of Molecular Hydrogen Under Pressure**
A. Ellis, S. Scott, A. Pandit, M. Miao. *Anticipated Submission December 2025*

[2] **Elucidation of α-Manganese Structure Under Increased Pressure**
A. Pandit, **A. Ellis**, S. Scott, M. Miao *Anticipated Submission December 2025*

[1] **Monolayer to Bulk Transition of Transition Metals**
A. Ellis, Y. Sun, M. Miao. *Anticipated Submission December 2025*

Presentations

- **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