

Austin Ellis

+1-818-384-4461 | austin.ellis.386@my.csun.edu |

 austinellis.org |  [LinkedIn](#) |  [GitHub](#) |  [ORCID](#) |

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.

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
 - Assisted new post-doc and undergraduate students in transition period by helping acclimate to relevant lab software and workflows
 - 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 (4x 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] **Batch Discovery of Complex Metal Superhydrides via an Effective Machine Learning Method Structured by Chemical Template Concept**
Yuanhui Sun, A. Ellis, X. Chen, M. Miao. *Journal of the American Chemical Society*. 2025. Accepted, in press. DOI: pending
- [3] **Pressure-induced Redox Reversal of Iron and the Distribution of Elements in Deep Earth**
X. Wang, X. Feng, J. Li, A. Ellis, S. Scott, D. Khodagholian, J. Lin, M. G. Jackson, F. J. Spera, S. A. T. Redfern, and M. Miao *Proceedings of the National Academy of Sciences*. 2025. Accepted, in press. DOI: pending
- [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 Electrifies 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. *Accepted by NeurIPS AI4Mat Conference September 2025*
- [1] **An Effective Machine Learning Frame for Materials Discovery Structured by a Chemical Concept**
Yuanhui Sun, A. Ellis, X. Chen, M. Miao. *Accepted by NeurIPS AI4Mat Conference September 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, M. Miao *Anticipated Submission December 2025*
- [1] **Monolayer to Bulk Transition of Transition Metals**
A. Ellis, 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 Leared 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 Laboratory 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
- **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
- **Chemistry Club Graduate Panel September, 2025:** Invited to speak at Chemistry Club panel to answer undergraduate questions about research in graduate school, and answer questions about the application process
- **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