

Samantha Ellis

NSF Graduate Research Fellow

Formerly publishing as Samantha Scott

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EDUCATION

• California State University, Northridge

Master of Science, Chemistry (GPA: 3.92)

Bachelor of Science, Chemistry (GPA: 3.77)

Northridge, USA
Expected Graduation Spring 2027
2024

• University of California, San Diego Extended Studies

Machine Learning Methods Certificate

Online
Expected December 2026

• University of California, Irvine

Completed coursework toward Bachelor of Science, Chemistry

Irvine, USA
2019–2020

• Fullerton College

Associate of Arts, Chemistry

Fullerton, USA
2019

RESEARCH EXPERIENCE

• Graduate Research Assistant, CSUN | Advisor: Maosheng Miao

January 2025 – Present

Realizing Pressure-Induced Cs 5p Core Reactivity in Cs Polyoxides

- Develop computational guidance for experimental target selection and spectroscopic identification of core-reactive Cs polyoxide phases under high pressure as the basis of my M.S. thesis in Chemistry.
- Identified spectroscopic signatures of pressure-induced Cs 5p core reactivity in CsO using XANES calculations to guide experimental diamond anvil cell studies.
- Built ternary Cs polyoxide convex hulls at 150 and 250 GPa to screen 35–45 candidate structures per hull and narrow experimentally viable reaction chemistries.
- Resolved Cs–O bonding changes in candidate core-reactive phases through projected density of states, Bader charge, and ICOHP analysis.

High-Pressure Redox Chemistry of Iron in Deep Earth Systems

- Mapped pressure-dependent phase stability across Fe–p-block compositions at 0, 150, and 300 GPa through CALYPSO structure searches and 25 HSE-based convex hulls.
- Quantified pressure-induced reversal of Fe redox behavior using HSE-based Bader charge analysis of 60 structures.
- Contributed to a co-authored *PNAS* publication on pressure-driven Fe redox reversal and deep-Earth element distribution.

Molecular Hydrogen Insulator-to-Metal Transition under High Pressure

- Characterized pressure-dependent band-gap closure and metallization in candidate molecular hydrogen phases using PBE and HSE band-structure calculations.
- Evaluated whether metallization can precede atomization through wavefunction-based analysis of the electronic character of compressed molecular hydrogen.
- Contributed to a manuscript in progress on the insulator-to-metal transition in molecular solid hydrogen and its implications for superconducting superhydrides.

• Research Student Internship, Oak Ridge National Laboratory

May 2026 – December 2026

Advisors: Eva Zarkadoula and Jingsong Huang

- Generate first-principles reaction data for fluorinated MoS₂ and WS₂ using VASP AIMD and on-the-fly MLFF-AIMD simulations.
- Curate chemically diverse data splits using t-SNE reaction embeddings and fine-tune separate MACE-MH-1 interatomic potentials.
- Reduce test energy errors from over 4,000 meV/atom to below 10 meV/atom and decrease force errors approximately fourfold.
- Validate temperature-dependent SF₃, MoF_x/WF_x, and pore-edge chemistry against reference molecular dynamics trajectories.
- Extend reactive simulations to systems with over 1,000 atoms and achieve approximately 480× greater sampling throughput than conventional AIMD.

• Undergraduate Research Assistant, CSUN | Advisor: Maosheng Miao

January 2024 – January 2025

- Conducted quantum-chemistry simulations on Linux-based HPC clusters using VASP and particle-swarm optimization to study electronic structure in solid-state systems.
- **Undergraduate Research Assistant, CSUN** | Advisor: Taeboem Oh January 2023 – January 2024
 - Supported multistep synthesis and NMR characterization of small organic molecules, including reaction setup and purification workflows.
- **Undergraduate Research Assistant, UCI** | Advisor: Sergey Nizkorodov December 2019 – December 2020
 - Optimized experimental protocols and novel SOA sampling devices to improve collection efficiency and data reliability.

PUBLICATIONS

- **Emerging Electride Behavior and Metallization in Molecular Hydrogen under High Pressure**
Ellis, A.; Ellis, S.; Pandit, A.; Miao, M. *J. Phys. Chem. Lett.* **2026**. DOI: [10.1021/acs.jpcclett.6c01415](https://doi.org/10.1021/acs.jpcclett.6c01415).
- **Pressure-Induced Redox Reversal of Iron and the Distribution of Elements in Deep Earth**
Wang, X.; Feng, X.; Li, J.; Lv, Y.; Ellis, A.; Scott, S.; Pandit, A.; Khodagholian, D.; Hemley, R. J.; Jackson, M. G.; Spera, F. J.; Redfern, S. A. T.; Miao, M. *Proc. Natl. Acad. Sci. U. S. A.* **2025**, 122(46), e2414911122. DOI: [10.1073/pnas.2414911122](https://doi.org/10.1073/pnas.2414911122).

MANUSCRIPTS UNDER REVISION

- **Prediction of Electron Localization Functions from Superposed Atomic Densities for Accelerated Superhydride Discovery**
Ellis, A.; Ellis, S.; Miao, M. *J. Mater. Inf.* **2026**, revisions submitted.

MANUSCRIPTS IN PROGRESS

- **Abnormal Behavior of Cs Polyoxides under High Pressure**
Sun, Y.; Khodagholian, D.; Ellis, S.; Ellis, A.; Miller, P.; Ji, C.; Gou, H.; Dronskowski, R.; Miao, M.
Manuscript in preparation.

SELECTED PRESENTATIONS

Oral Presentations:

- **S. Ellis:** *Pressure-induced Redox Reversal of Iron and the Distribution of Elements in Deep Earth.*
2026 CSUN Research and Creative Works Symposium (CSUNposium), Northridge, CA, April 2026.
- **S. Scott:** *Pressure-induced Redox Reversal of Iron and the Distribution of Elements in Deep Earth.*
2026 American Physical Society Global Summit (APS), Denver, CO, March 2026.
- **S. Scott:** *Pressure-induced Redox Reversal of Iron and the Distribution of Elements in Deep Earth.*
2025 CSUN Sigma Xi Research Symposium, Northridge, CA, December 2025.

Poster Presentations:

- **S. Ellis, M. Lee, J. Huang, and E. Zarkadoula:** *Modeling Gas-Assisted Etching of MoS₂ and WS₂ with Machine-Learned Interatomic Potentials.*
2026 Oak Ridge Institute for Science and Education (ORISE) Symposium, Oak Ridge, TN, July 2026.
- **S. Ellis, Y. Sun, A. Ellis, X. Chen, M. Miao:** *An Effective Machine Learning Frame for Materials Discovery Structured by a Chemical Concept.*
2025 NeurIPS AI4Mat Workshop, San Diego, CA, December 2025.
- **S. Scott, A. Ellis, A. Pandit, and M. Miao:** *Insulator to Metal Transition of Molecular Hydrogen Under Pressure.*
2025 CSUN Research and Creative Works Symposium (CSUNposium), Northridge, CA, April 2025.
- **S. Scott, A. Ellis, A. Pandit, and M. Miao:** *Insulator to Metal Transition of Molecular Hydrogen Under Pressure.*
2025 American Physical Society Global Summit (APS), Anaheim, CA, March 2025.

Co-authored Presentations:

- **A. Ellis, S. Scott, and M. Miao:** *Seitz-Invariant Prediction of Electron Localization Functions from Superposed Atomic Densities via a 3D-Convolutional Network.*
2026 American Physical Society Global Summit (APS), Denver, CO, March 2026.
- **A. Pandit, A. Ellis, S. Scott, and M. Miao:** *Interactions that Govern the Structure of α -Manganese.*
2025 American Physical Society Global Summit (APS), Anaheim, CA, March 2025.

TEACHING EXPERIENCE

- **Teaching Assistant - General Chemistry and Organic Chemistry Labs, CSUN** January 2025 – May 2026
 - Taught two General Chemistry laboratory sections for 2 semesters, guiding 24 students per section in solution preparation, titration, electrochemistry, and quantitative analysis.

- Taught two Organic Chemistry laboratory sections for 1 semester, guiding 18 students per section in synthesis, purification, spectroscopic analysis, and mechanistic interpretation.
- Developed and deliver prelaboratory lectures, problem-solving sessions, and safety briefings aligned with course learning objectives.
- Trained students in rigorous notebook practice, including procedural documentation, calculations, and observational quality control.
- Incorporated scientific literature and research-oriented thinking into laboratory instruction through structured extracurricular assignments.

MENTORING AND OUTREACH

- **Journal Coordinator - CSUN ACS Chemistry and Biochemistry Club** *August 2025 – May 2026*
 - Co-founded and coordinate CSUN's monthly Journal Club spanning chemistry and biochemistry, including article selection, presenter scheduling, and event logistics.
 - Developed participants' scientific reading and communication skills through structured discussion, figure analysis, and presentation feedback.
 - Supported early undergraduate mentorship by pairing students with graduate facilitators and connecting interested participants with research labs and opportunities.
- **Graduate Peer Mentor - Office of Undergraduate Research, CSUN** *June 2025 – May 2026*
 - Lead three weekly student-facing workshops reaching 30–45 students on research onboarding, graduate applications, conference preparation, and professional development.
 - Provided weekly one-on-one advising on joining research labs, drafting SOPs and personal statements, preparing abstracts and posters, and developing CVs and resumes.
 - Facilitated undergraduate research programs, including mentor-matching events such as Getting Into Research.
 - Designed a two-week summer course in computational drug discovery for 12 undergraduates, introducing protein structure-based drug design, molecular docking, molecular dynamics, and AI-assisted workflows, scheduled to launch in June 2026.

INDUSTRY EXPERIENCE

- **Research and Development Lab Technician - New Look Cosmetics, Chatsworth** *May 2022 – January 2024*
 - Managed 3–5 concurrent projects and collaborated with engineers to scale validated formulations from laboratory to pilot production.
 - Designed, optimized, and troubleshooted formulation experiments with chemists using quantitative and analytical problem-solving methods.
 - Maintained electronic formulation and project-management records to support reproducibility and data integrity.

HONORS AND AWARDS

- **National Science Foundation Graduate Research Fellowship (NSF GRFP)** *2026*
National Science Foundation
- **Leslie and Terry Cutler Scholarship** *2026*
College of Science and Mathematics, CSUN
- **Dr. Frank Harris Graduate Scholarship Endowment in Chemistry and Biochemistry** *2026*
Department of Chemistry and Biochemistry, CSUN
- **Outstanding Achievement Award** *2026*
Department of Chemistry and Biochemistry, CSUN
- **Outstanding Leadership Award** *2026*
Department of Chemistry and Biochemistry, CSUN
- **Second Place, Sigma Xi Research Symposium** *2025*
Sigma Xi Research Society, CSUN
- **Dr. Lan K. Wong Undergraduate Research Award - \$1000** *2022*
Department of Chemistry and Biochemistry, CSUN
- **ACS Undergraduate Award in Organic Chemistry** *2022*
Department of Chemistry and Biochemistry, CSUN
- **Michael E. Gebel Award** *2020*
Department of Chemistry, UCI

SKILLS

- **Computational Methods:** density functional theory, crystal-structure prediction, convex-hull construction, bonding analysis, IR/XANES simulation
- **Software:** VASP, Quantum ESPRESSO, CALYPSO, LOBSTER, Bader analysis, FEFF, OVITO
- **Programming:** Python, PyTorch, TensorFlow, NumPy, Pandas
- **High-Performance Computing:** Linux/Unix, parallel workflows, GPU computing
- **Scientific Communication:** LaTeX, scientific writing, workshop development, peer mentorship

RELEVANT GRADUATE COURSEWORK

- **GEOL 502/L Scanning Electron Microscopy with Lab:** SEM instrumentation, sample preparation, SE/BSE imaging, EDS mapping, introductory EBSD
- **CHEM 543/595S Chemistry of Energy with Lab:** batteries, fuel cells, supercapacitors, hydrogen systems, photovoltaics, electrochemical characterization
- **CHEM 534 Advanced Organic Chemistry:** physical organic chemistry, kinetics, thermodynamics, catalysis, and mechanism analysis