

Alexander M. Chang

Email: achang67@stanford.edu
Department of Chemistry | Stanford University

EDUCATION

- 2019 – Present **Stanford University** | Stanford, CA
Ph.D. | Theoretical Chemistry
Research Advisor: Prof. Todd J. Martínez
- 2015 – 2019 **Yale University** | New Haven, CT
B.S. | Chemistry, Applied Mathematics (Distinction in both Majors)
Research Advisor: Prof. Victor S. Batista
Cumulative GPA: 3.80/4.00

AWARDS & HONORS

- 2023 Linus Pauling Teaching Award
Stanford University – Department of Chemistry
- 2021 – 2024 National Science Foundation Graduate Research Fellowship
National Science Foundation
- 2020 Outstanding Graduate Student Poster – Virtual Conference of Theoretical Chemistry 2020
- 2019 – 2022 Stanford Graduate Fellowship in Science and Engineering
Stanford University – Department of Chemistry
- 2019 Arthur Fleischer Award (for Outstanding Performance in Chemistry)
Yale University – Department of Chemistry
- 2016 Yale College Freshman Summer Research Fellowship
Yale University

TEACHING & OUTREACH

- Fall 2023 Center for Teaching and Learning Teaching Advancement Grant
- Designing lab for Chem 31A (General Chemistry) that integrates Interactive Molecular Dynamics in virtual reality into curriculum
 - Acquired grant money and partnered with Stanford Virtual Human Interaction Lab to supply Oculus VR headsets for students
- 2023 – Stanford Jail & Prison Education Project
- Designed course with team of co-lecturers for inmates in San Francisco jail
 - Gave lectures on chemical bonding adapted for jail classroom (*e.g.* no electronics)
- Spring 2023 Splash
- Taught high schoolers chemistry using interactive molecular dynamics in virtual reality
- Fall 2022 Chem 31A (General Chemistry) Head Teaching Assistant
- Managed day-to-day logistics for 300-student course
 - Led team of first-year TAs, delegated their duties and organized office hour/lab schedules

- Helped create exams and write answer key as well as design novel questions for students
 - Ran grading sessions of TAs and mercenary graders for three midterms and final exam
- 2021 – 2023 Stanford Future Advancers of Science and Technology (FAST) Mentor
- 2021-2022: Designed machine learning project for student to predict Amazon booksales
 - Helped student learn how to code in python via weekly Saturday FAST sessions
 - 2022-2023: Designed math-based freezing point depression project for student
 - Tailored experimental design to fit student's interest in calculus
- Summer 2021 Martinez Group Summer School Lecturer
- Gave 3-hour lecture on enhanced sampling methods for free energy calculations
 - Created and graded homework assignments based on lecture material
- Fall 2020 Chem 33 (Organic Chemistry) Teaching Assistant | Stanford University
- Served as Exam TA: helped make, vet, and grade 8 quizzes and 2 exams
 - Held 6 office hours a week
 - Guided students through practice problems in breakout rooms during lectures
- 2019, 2021-2023 Mercenary Grader for General Chemistry
- Graded midterms and final exam for Stanford general chemistry classes
- 2019 Yale Young Global Scholars Instructor | Yale University
- Guided high schoolers on their own machine learning research projects
 - Created/gave seminars on probability, machine learning, research ethics, and geophysics
 - Led discussion sections on lectures by Yale faculty
- 2018 Center for Teaching and Learning Science & QR Tutor | Yale University
- Tutored freshmen each for 1 hr/week in organic chemistry
- 2015 – 2016 MathCounts Outreach Instructor | Nathan Hale School, New Haven CT
- Created lecture plans and led group sessions for MathCounts

PUBLICATIONS

05. Efficient Acceleration of Reaction Discovery in the *Ab Initio Nanoreactor*: Phenyl Radical Oxidation Chemistry
Chang, A. M.; Meisner, J.; Xu, R.; Martínez, T. J., *Journal of Physical Chemistry A*, **2023**, DOI: [10.1021/acs.jpca.3c05484](https://doi.org/10.1021/acs.jpca.3c05484)
04. First Principles Reaction Discovery: From the Schrodinger Equation to Experimental Prediction for Methane Pyrolysis
 Xu, R.; Meisner, J.; **Chang, A. M.**; Thompson, K. C.; Martínez, T. J., *Chem. Sci.* **2023**
03. The non-adiabatic nanoreactor: towards the automated discovery of photochemistry
 Pieri, E.; Lahana, D.; **Chang, A. M.**; Aldaz, C. R.; Thompson, K. C.; Martínez, T. J., *Chem. Sci.* **2021**
02. Hammett Neural Networks: Prediction of Frontier Orbital Energies of Tungsten-Benzylidyne Photoredox Complexes
Chang, A. M.; Freeze, J. G.; Batista, V. S., *Chem. Sci.*, **2019**, *10*, 6844-6854.
01. Inverse Design of a Catalyst for Aqueous CO/CO₂ Conversion Informed by the Ni^{II}-iminothiolate Complex
Chang, A. M.; Rudshiteyn, B.; Batista, V. S., *Inorg. Chem.* **2018**, *57* (24), 15474-15480.

RESEARCH

- 2019 – Present Graduate Student, Stanford University | Advisor: Prof. Todd J. Martínez
- Developing and applying *ab initio* nanoreactor framework and codebase
 - Created novel reaction discovery methods for accelerated molecular dynamics
 - Analyzed and compared efficiencies and biases of various reaction-accelerating forces
- 2017 – 2019 Undergraduate Researcher, Yale University | Advisor: Prof. Victor S. Batista
- Used a tight-binding linear combination of atomic potentials (TB-LCAP) inverse design to discover optimal nickel catalysts for CO oxidation; ran density functional theory (DFT) calculations on catalytic cycle, including relaxed scans and transition state calculations.
 - Developed novel neural network methodology using Hammett parameters to describe ligands of tungsten catalyst for molecular design; employed machine learning techniques to examine data and hypothesize chemical theory behind mathematical trends.
 - Created inverse design gradient descent algorithm using neural network scoring function to optimize catalyst ligands for reductive power
- Summer 2016 Undergraduate Researcher, Yale University | Advisor: Prof. Seth Herzon
- Aided in synthesis of precolibactins

POSTER PRESENTATIONS

- 2023 West Coast Conference on Theoretical Chemistry | Davis, CA
- 2022 American Conference on Theoretical Chemistry | Olympic Valley, CA
- 2021 Bay Area Theoretical Chemistry Virtual Poster Session
- 2020 Virtual Conference of Theoretical Chemistry 2020
- 2019 257th ACS National Meeting | Orlando, FL
- 2018 Boston University Cokerfest Symposium | Boston, MA

SKILLS

- Language/Script: Python, R, Bash, LaTeX, C
- Programs: VMD, Gaussian, TeraChem, Avogadro, Keras/TensorFlow, ChemDraw, Excel, Prism

LEADERSHIP & VOLUNTEER EXPERIENCES

- 2020 – 2021 Student Affairs Committee for Chemistry Department | Stanford University
- 2016 – 2018 Volunteers Around the World Yale Chapter | Peru; Dominican Republic
2017 – 2018 Team Co-Leader and Head of Finances
- 2015 – 2019 Davenport Pops Orchestra | Yale University
2017 – 2018 Director of Development | 2016 – 2017 Treasurer