

SAMUEL D. YOUNG

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EDUCATION

University of Michigan, College of Engineering (Ann Arbor, MI) **Aug 2023**
Ph.D. in Chemical Engineering

- Degree awarded August 18, 2023. Advised by Prof. Bryan R. Goldsmith.
- Dissertation title: “Heterogeneous Electrocatalysts for Aqueous Nitrate Reduction and Nitrogen Chemistry”.
- Cumulative GPA: 4.00/4.00.
- Research themes: nitrate reduction, water purification, heterogeneous catalysis, materials science.
- 2018–2019 Fellow of the Michigan Institute for Computational Discovery and Engineering.
- 2022–2023 J. Robert Beyster Computational Innovation Graduate Fellow.

University of Michigan, College of Engineering (Ann Arbor, MI) **Dec 2020**
Master of Science in Chemical Engineering

- Cumulative GPA: 4.00/4.00.
- Three-time recipient of a research computing allocation from the National Energy Research Scientific Computing Center (NERSC), totaling 2.75M service units.

Cornell University, College of Engineering (Ithaca, NY) **May 2016**
Bachelor of Science in Chemical Engineering

- Graduated *magna cum laude* (cumulative GPA: 3.86/4.00).
- John McMullen Scholar.
- Three-time recipient of a Semiconductor Research Corporation research grant.

RESEARCH EXPERIENCE

U.S. Army DEVCOM Army Research Laboratory (Adelphi, MD) **2024–Current**
Distinguished Postdoctoral Fellow (Energy Sciences)

- Current research focus is on computational simulation of 3 dense ionic battery electrolyte chemistries for beyond-Li battery applications, as well as small organic molecules for novel aqueous electrolytes.
- Conducted 15 Born–Oppenheimer molecular dynamics simulations, showing that Li–Cl electrolyte chemistries suffer from slow transport kinetics when paired with heavy transition metal ions.
- Performed 650 density functional theory calculations to study the adsorption of small, N-containing molecules to iron electrodes, finding that such molecules may poison the electrode surface in aqueous conditions.
- Trained 60 equivariant, deep neural network machine learning models as candidate interatomic potentials to accelerate molecular dynamics calculations by factors of 10–1000.
- Authored a user guide on remote development using Visual Studio Code for the DoD High Performance Computing Modernization Project user community of approximately 4000 users across 8 supercomputers.

University of Michigan (Ann Arbor, MI) **2018–2024**

- Developed a web app and graph database for 10–100 monthly active users to document complex metal alloy synthesis recipes, alloy characterization data, and experimentally measured alloy material properties.
- Conducted an exhaustive DFT study of over 900 simulations to understand nitrate reduction on platinum–ruthenium alloys. Found that alloys of approximate composition $\text{Pt}_{75}\text{Ru}_{25}$ best remove nitrate from polluted water sources.
- Studied the vacuum-phase stability and poison resistance of rhodium sulfide surfaces using DFT. Found that S-defected rhodium sulfide surfaces display partial resistance to chloride poisoning in water and identified $\text{Rh}_3\text{S}_4(100)$ as an active phase for nitrate reduction.

- Mentored two graduate students, three undergraduate students, and a master's student in density functional theory, machine learning, and materials informatics screening, leading to a machine learning model for predicting chemisorption on metal alloys.

Los Alamos National Laboratory (Los Alamos, NM)

2021

- Conducted a screening study of 295 perovskite oxynitride compounds to understand which factors influence the formability of these compounds, leading to a paper in *ACS Chemistry of Materials*.
- Published two first-author perspective articles for *Trends in Chemistry* and *Journal of Physical Chemistry C*, focusing on metal oxynitrides as tunable materials for electrocatalytic ammonia synthesis.

U.S. Army Edgewood Chemical Biological Center (Edgewood, MD)

2017–2018

- Synthesized and characterized the structure of PCN-222, UiO-66, and UiO-67 (MOF) catalysts identified for possible activity against chemical warfare agents. Characterized the kinetics of photocatalytic nerve agent simulant decomposition in the presence of PCN-222.

INDUSTRY EXPERIENCE

U.S. Army Edgewood Chemical Biological Center (Edgewood, MD)

2016–2018

- Developed a Microsoft Access database application to track progress of Army unit chemical detector equipment upgrades, including dependency resolution, rapid data input, and compliance reporting.
- Managed routine testing of 134 air compressors across 59 active-duty, Reserve, and National Guard Army units. Developed a Microsoft Access database application to track tests and produce compliance reports.
- Collaborated with the Japan Ministry of Defense to design and manufacture a new chemical detector, including attending 3 face-to-face conferences, coordinating two months of testing, and planning over 450 test trials.

DEPARTMENT AND COMMUNITY SERVICE

University of Michigan (Ann Arbor, MI)

2019-current

- Served as chair for the Chemical Engineering department-wide graduate symposium. The symposium showcases current students' work, leads to hiring opportunities, and strengthens the department's relationships with industry partners.
- Adjudicated an undergraduate poster session and provided feedback to help students improve their scientific communication skills.

U.S. Army Edgewood Chemical Biological Center (Edgewood, MD)

2017

- Adjudicated 2 science fairs at Cecil County public schools. Provided feedback to 16 students to help raise interest in STEM fields.

TEACHING EXPERIENCE

University of Michigan (Ann Arbor, MI)

2019–2021

ChE 505 – Applied Mathematics for Chemical Engineering

Fall 2021

- Served as a graduate student instructor for 32 students. Wrote 9 homework assignments, proctored and graded 2 exams, held weekly office hours, and designed and facilitated a semester capstone project.
- Developed grading standards and procedures to ensure fair grading across all students and assignments.

ENGR 1000-320 – Practical Data Science for Engineers

Fall 2020

- Served as a graduate student instructor for a class of 44 students to help teach a data science course with an emphasis on machine learning. Responsibilities included facilitating laboratory exercises for 2 sections of 22 students each, holding weekly office hours, and grading homework.
- Created a Python framework to automate grading group assignments, including rapid data entry via Google Forms and integration with Canvas LMS, shortening our grading turnaround to 3 days instead of a week.

ChE 505 – Applied Mathematics for Chemical Engineering

Fall 2020

- Served as a graduate student instructor for a class of 41 students. Composed 9 homework assignments, proctored and graded 2 exams, held biweekly office hours, and conducted one-on-one student mentoring.

- Helped teach a class of 12 undergraduate students a lecture about machine learning in March 2019. Developed a laboratory assignment and held office hours to help students practice basic machine learning.

LEADERSHIP EXPERIENCE

University of Michigan (Ann Arbor, MI) 2019–current

- Mentored three undergraduate students in density functional theory, machine learning, and high-throughput screening for materials informatics, leading to a preliminary machine learning model for predicting chemisorption on metal alloys.
- Mentored a master's student on applying crystal graph convolutional neural network models to chemisorption energy prediction.

U.S. Army Edgewood Chemical Biological Center (Edgewood, MD) 2017–2018

- Trained 2 employees to perform major responsibilities within 3 active projects in our branch, including preparing 40 pages of training documentation, creating 4 standard operating procedures, and running 3 live training sessions to teach other members of my team.
- Helped select 4 new contractor employees for our team, including offering informational interviews, touring candidates around the workplace, and assisting in the interview process.
- Planned social and recreational activities to help new employees feel welcome.

PUBLICATIONS

- Samuel D. Young, Jiadong Chen, Wenhao Sun, Bryan R. Goldsmith, Ghanshyam Pilania. Thermodynamic Stability and Anion Ordering of Perovskite Oxynitrides. *Chemistry of Materials* **2023**, 35 (15), 5975–5987. <https://doi.org/10.1021/acs.chemmater.3c00943>.
- Samuel D. Young, Bianca Ceballos, Amitava Banerjee, Rangachary Mukundan, Ghanshyam Pilania, Bryan R. Goldsmith. Metal Oxynitrides for the Electrocatalytic Reduction of Nitrogen to Ammonia. *Journal of Physical Chemistry C* **2022**, 126 (31), 12980–12993. <https://doi.org/10.1021/acs.jpcc.2c02816>. **Selected as an ACS Editors' Choice article.**
- Danielle Richards, Samuel D. Young, Bryan R. Goldsmith, Nirala Singh. Electrocatalytic nitrate reduction on rhodium sulfide compared to Pt and Rh in the presence of chloride. *Catalysis Science & Technology* **2021**, 11 (22), 7331–7346. <https://doi.org/10.1039/d1cy01369f>.
- Samuel D. Young, Amitava Banerjee, Ghanshyam Pilania, Bryan R. Goldsmith. Perovskite Oxynitrides as Tunable Materials for Electrocatalytic Nitrogen Reduction to Ammonia. *Trends in Chemistry* **2021**, 3 (9), 694–696. <https://doi.org/10.1016/j.trechm.2021.07.002>.
- Zixuan Wang, Samuel Young, Bryan Goldsmith, Nirala Singh. Increasing Electrocatalytic Nitrate Reduction Activity by Controlling Adsorption through PtRu Alloying. *Journal of Catalysis* **2021**, 395, 143–154. <https://doi.org/10.1016/j.jcat.2020.12.031>.
- James R. O'Dea, Megan Holtz, Anna Legard, Samuel Young, *et al.* Conductivity and Microstructure of Combinatorially Sputter-Deposited Ta–Ti–Al Nitride Thin Films. *Chemistry of Materials* **2015**, 27 (13), 4515–4524. <https://doi.org/10.1021/cm504599s>.

CONFERENCE TALKS AND POSTERS

- Samuel D. Young. “Heterogeneous Electrocatalysts for Aqueous Nitrate Reduction and Nitrogen Chemistry”. U.S. Army Research Lab Distinguished Postdoctoral Fellowship Candidate Seminar, 12 Oct 2023. Virtual. *Invited seminar as a Distinguished Postdoctoral Fellowship finalist.*
- Samuel D. Young, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. “Thermodynamic Stability and Anion Ordering in ABO₂N and ABON₂ Perovskite Oxynitrides”. 44th Annual Symposium of the Michigan Chapter of the North American Catalysis Society, 16 May 2023. Ann Arbor, MI, United States.
- Samuel D. Young, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. “Thermodynamic Stability and Anion Ordering in ABO₂N and ABON₂ Perovskite Oxynitrides”. 2022 AIChE Annual Meeting, 18 Nov 2022. Phoenix, AZ, United States.

- Samuel D. Young, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. “Thermodynamic Stability and Anion Ordering in ABO_2N and ABON_2 Perovskite Oxynitrides”. 43rd Annual Symposium of the Michigan Chapter of the North American Catalysis Society, 04 Oct 2022. Midland, MI, United States.
- Samuel D. Young, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. “Thermodynamic Stability and Anion Ordering in ABO_2N and ABON_2 Perovskite Oxynitrides”. University of Michigan Fall 2022 Chemical Engineering Graduate Symposium, 22 Sep 2022. Ann Arbor, MI, United States. *Presentation awarded 3rd place of 15 oral presenters.*
- Samuel D. Young, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. “Thermodynamic Stability and Anion Ordering in ABO_2N and ABON_2 Perovskite Oxynitrides”. ACS Fall 2022 Meeting, 23 Aug 2022. Chicago, IL, United States.
- Zixuan Wang, Samuel D. Young, Nirala Singh, Bryan Goldsmith. “Platinum-Ruthenium Alloys As Electrocatalysts for Efficient Aqueous Nitrate Reduction”. 2021 AIChE Annual Meeting, 16 Nov 2021. Virtual.
- Danielle Richards, Samuel Young, Nirala Singh, Bryan Goldsmith. “Rhodium Sulfide Electrocatalysts for Electrocatalytic Nitrate Reduction”. ACS Fall 2021 Meeting, 26 August 2021. Virtual.
- Zixuan Wang, Samuel Young, Nirala Singh, Bryan Goldsmith. “Platinum-Ruthenium Alloys as Electrocatalysts for Efficient Aqueous Nitrate Reduction”. ACS Spring 2021 Meeting, 13 April 2021. Virtual.
- Samuel Young, Jin-Xun Liu, Zixuan Wang, Danielle Richards, Nirala Singh, Bryan Goldsmith. “Understanding Metal Alloys and Rhodium Sulfides as Electrocatalysts for Nitrate Reduction” (poster), August 2019. University of Barcelona, Barcelona, Spain.
- Samuel Young, Ryan Dwyer, John Marohn. “Interferometric Measurement of Thin-Film Corrosion in Fuel Cell Materials” (poster). Cornell University, April 2016. Ithaca, NY, United States.

SKILLS

- **High-throughput computing:** Slurm, Lmod, PBS/Torque, Fireworks.
- **Data science, machine learning:** Python (NumPy, SciPy, Matplotlib, Pandas, scikit-learn), MATLAB, Excel.
- **Web development:** React, Vite, Django, Node.js, Tailwind CSS, PostCSS, SWR, Rancher, Insomnia, Hoppscotch.
- **Cloud computing:** Docker, docker-compose, Kubernetes, Rancher, Let’s Encrypt.
- **Scripting:** Python, Bash, PowerShell, Visual Basic for Applications (VBA).
- **Databases:** MongoDB (PyMongo), PostgreSQL, JET SQL, Microsoft Access (VBA+DAO interface).
- **Atomistic modeling:** LAMMPS, NequIP/Allegro, DeePMD-kit v2, Atomic Simulation Environment, Pymatgen, Vienna Ab Initio Simulation Package.
- **Chemical characterization:** FTIR, UV-Vis, PXRD, tapping and conductive-probe AFM.