

# SAMUEL D. YOUNG

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## EDUCATION

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**University of Michigan, College of Engineering (Ann Arbor, MI)** **2018–Current**  
***Ph.D. Candidate in Chemical Engineering***

- Fourth-year student in the Goldsmith Computational Modeling Laboratory. Currently using black-box and interpretable machine learning tools and density functional theory (DFT, a quantum-mechanical computational approach) to build active machine learning workflows for catalyst discovery. Also conducting research on perovskite oxynitride reactivity toward electrocatalytic nitrate reduction.
- 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: 3.83/4.00).
- John McMullen Scholar.
- Three-time recipient of a Semiconductor Research Corporation research grant.
- Extracurricular activities: Cornell University Symphonic Band.

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## RESEARCH EXPERIENCE

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

- Currently developing convolutional neural network and explainable boosting machine machine-learning models to understand how experimental synthesis conditions correlate to metal alloy activity and stability.
- 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 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 high-throughput screening study of 295 perovskite oxynitride compounds to understand which factors influence the formability of these compounds.
- Published a first-author invited Forum article for *Trends in Chemistry* focusing on perovskite oxynitrides as tunable materials for electrocatalytic ammonia synthesis.

**U.S. Army Edgewood Chemical Biological Center (Edgewood, MD)** **2017–18**

- Synthesized and characterized the structure and reactivity of 2 metal organic framework (MOF) catalysts identified for possible activity against toxic chemical agents.

**Cornell University (Ithaca, NY)****2012–13, 2015–16**

- Completed preliminary development of a laser interferometer to monitor real-time fuel cell corrosion growth, including a LabVIEW-based data acquisition and control system.
- Imaged over 70 regions of nitride thin film samples with conductive probe atomic force microscopy (cp-AFM) to identify a robust fuel cell catalyst support material, leading to an article in *Chemistry of Materials*.

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**INDUSTRY EXPERIENCE**

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**U.S. Army Edgewood Chemical Biological Center (Edgewood, MD)****2016–18**

- 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.

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**DEPARTMENT AND COMMUNITY SERVICE**

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**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.

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**TEACHING EXPERIENCE**

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**University of Michigan (Ann Arbor, MI)****2019-current***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 the Canvas gradebook. Enabled us to grade projects in 3 days rather than a week.

*ChE 505 – Applied Mathematics for Chemical Engineering**Fall 2020*

- Served as a graduate student instructor for a class of 41 students. Responsibilities included writing 9 homework assignments, proctoring and grading 2 exams, holding weekly office hours, and one-on-one student mentoring.

*ChE 496 – Advanced Special Topics in Chemical Engineering**March 2019*

- 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.

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## LEADERSHIP EXPERIENCE

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### 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.
- Currently mentoring 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.

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## PUBLICATIONS

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- 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>.

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## CONFERENCE TALKS AND POSTERS

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- Samuel D. Young, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. “Thermodynamic Stability and Anion Ordering in ABO<sub>2</sub>N and ABON<sub>2</sub> 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.

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## SKILLS

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- **High-throughput computing:** Slurm, PBS/Torque, Fireworks
- **Data analysis and Machine Learning:** Python (NumPy, SciPy, Matplotlib, Pandas, scikit-learn), MATLAB, Microsoft Excel, LabVIEW
- **Web development:** React, Django, Node.js, Tailwind CSS, PostCSS, SWR, Rancher
- **Databases:** MongoDB (PyMongo), PostgreSQL, JET SQL, Microsoft Access (VBA, DAO interfaces)
- **Scripting:** PowerShell, Visual Basic for Applications (VBA), Python, Bash
- **Atomistic modeling:** Atomic Simulation Environment, Pymatgen, Vienna Ab Initio Simulation Package
- **Chemical characterization:** FTIR, UV-Vis, PXRD, tapping and conductive probe AFM