SAMUEL D. YOUNG

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EDUCATION

University of Michigan, College of Engineering (Ann Arbor, MI)   **2018–Current**
Ph.D. Candidate in Chemical Engineering
- Third-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.
- 2018–2019 Fellow of the Michigan Institute for Computational Discovery and Engineering

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

RESEARCH EXPERIENCE

University of Michigan (Ann Arbor, MI)   **2018–Current**
- Currently developing algorithmic workflows using active machine learning to study effective nitrate reduction alloy electrocatalysts for wastewater remediation.
- Performed 1837 DFT calculations on bimetallic alloys of 5 metals and am currently training a crystal graph convolutional neural network to predict adsorbate binding energies.
- Conducted an exhaustive DFT study of 108 simulations to predict how strongly nitrogen and oxygen atoms bind on platinum-ruthenium alloys. The results support trends observed by our experimental collaborators.
- Studied the vacuum-phase stability of rhodium sulfide surfaces using DFT. Conducted 26 simulations to predict which surfaces are most stable. This is the first known prediction of these stable surfaces.

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*.

INDUSTRY EXPERIENCE

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.

DEPARTMENT AND COMMUNITY SERVICE

University of Michigan (Ann Arbor, MI)   **2019-current**
- Current chair on the committee that plans each year's department-wide chemical engineering 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-current**
- Currently a graduate student instructor in the Winter 2021 semester for ENGR 100: Introduction to Engineering, with an emphasis on machine learning. Responsibilities include facilitating laboratory exercises for 2 sections of 22 students each, holding weekly office hours, and grading homework.
- Served as a graduate student instructor in the Fall 2020 semester for ChE 505: Applied Mathematics for Chemical Engineering, 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.
- 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.
- 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.

PUBLICATIONS

- Zixuan Wang, <u>Samuel Young</u>, Nirala Singh, Bryan Goldsmith. 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.
- Danielle Richards, <u>Samuel Young</u>, Nirala Singh, Bryan Goldsmith. Electrocatalytic Nitrate Reduction on Pt/C, Rh/C, and Rh_xS_y/C: Effect of Chloride. Unpublished work.
- James R. O'Dea, Megan Holtz, Anna Legard, <u>Samuel Young</u>, *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

- <u>Samuel Young</u>, Jin-Xun Liu, Zixuan Wang, Danielle Richards, Nirala Singh, Bryan Goldsmith. "Understanding Metal Alloys and Rhodium Sulfides as Electrocatalysts for Nitrate Reduction". Poster presentation given at University of Barcelona, August 2019.
- <u>Samuel Young</u>, Ryan Dwyer, John Marohn. "Interferometric Measurement of Thin-Film Corrosion in Fuel Cell Materials". Poster presentation given at Cornell University, April 2016

SKILLS

- **High-throughput computing**: Slurm, PBS/Torque
- **Data analysis and Machine Learning**: Python (NumPy, SciPy, Matplotlib, Pandas, scitkit-learn), MATLAB, Microsoft Excel, LabVIEW
- **Databases**: MongoDB (PyMongo), 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