Samuel D. Young, Ph.D.

Computational Chemistry Researcher | Density Functional Theory | Molecular Dynamics | Python | Linux

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📍 **Adelphi, MD**

EDUCATION

Ph.D. in Chemical Engineering
University of Michigan

📅 Aug 2023　　📍 Ann Arbor, MI

- Advisor: Professor Bryan R. Goldsmith.
- Dissertation title: "Heterogeneous Electrocatalysts for Aqueous Nitrate Reduction and Nitrogen Chemistry".
- Cumulative GPA: 4.00/4.00.
- 2018–2019 Fellow of the Michigan Institute for Computational Discovery and Engineering.
- 2022–2023 J. Robert Beyster Computational Innovation Graduate Fellow.
- Research themes: atomistic materials modeling, bulk liquid simulation, microkinetic reaction modeling, nitrate reduction, energy storage, water purification, heterogeneous catalysis.

M.S. in Chemical Engineering
University of Michigan

📅 Dec 2020　　📍 Ann Arbor, MI

- 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.

B.S. in Chemical Engineering
Cornell University

📅 May 2016　　📍 Ithaca, NY

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

SKILLS

- **Atomistic modeling**: Atomic Simulation Environment, Pymatgen, VASP, CP2K, LAMMPS, NequIP/Allegro, DeePMD-kit v2.
- **Programming**: Python, basic C++, Bash, PowerShell, Visual Basic for Applications (VBA).
- **High-throughput computing**: Slurm, Lmod, PBS/Torque, Fireworks, OpenMP.
- **Data science, machine learning**: Python (NumPy, SciPy, Matplotlib, Pandas, scitkit-learn, PyTorch), MATLAB.
- **Cloud computing**: Docker, docker-compose, Kubernetes, Rancher, Let's Encrypt.
- **Web development:** React, Vite, Django, Node.js, Tailwind CSS, PostCSS, SWR, react-chartjs-2, Rancher, Insomnia, Hoppscotch.
- **Databases**: MongoDB (PyMongo), PostgreSQL, JET SQL, Microsoft Access (VBA+DAO interface).
- **Linux distro familiarity**: SLES, CentOS/Rocky/RHEL (user); Ubuntu, OpenSUSE, Arch Linux (admin, daily driver).

RESEARCH EXPERIENCE

Distinguished Postdoctoral Fellow (Energy Sciences)
U.S. Army DEVCOM Army Research Laboratory

📅 2024–present　　📍 Adelphi, MD

- Currently parameterizing equivariant, transformer-based graph neural network models to accelerate molecular dynamics (MD) simulations of Li and beyond-Li dense ionic liquid electrolytes, including Li–Zn–Cl and Li–Mn–Cl systems.
- Conducted a large-scale campaign of ~11,000 geometry relaxations to study adsorption of N-containing compounds to iron electrodes using the DFT-trained EquiformerV2 model, finding that such molecules may alter the surface-electrolyte interface in aqueous conditions and hamper charge transfer.
- Developed a Python library for rapidly designing, executing, and post-processing pipelines of hundreds of geometry relaxations or molecular dynamics calculations in VASP and CP2K, including directed acyclic graphs of tasks for each calculation.
- Authored a user guide on remote development using Visual Studio Code for the DoD High Performance Computing Modernization Project user community of approximately 4,000 users across 8 Linux supercomputers.

Graduate Student, Postdoctoral Associate
University of Michigan

📅 2018–2024 📍 Ann Arbor, MI

- Conducted an exhaustive density functional theory study of over 900 simulations to understand nitrate reduction on Pt–Ru alloys. Found that alloys of approximate composition $Pt_{75}Ru_{25}$ best remove nitrate from polluted water sources.
- Developed a web app and graph database for 10–100 monthly active users to document complex metal alloy synthesis recipes, characterization data, and material properties that may ultimately power structure-property AI models for inverse alloy design.
- 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 $Rh_3S_4(100)$ as an active phase for nitrate reduction.
- Mentored 2 graduate students, 3 undergraduate students, and 1 master's student in density functional theory, machine learning, and materials informatics screening, leading to potential future collaboration on a computer vision model for predicting chemisorption of small organic molecules on metal alloys.

Visiting Graduate Student Scientist
Los Alamos National Laboratory

📅 2021 📍 Los Alamos, NM

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

Chemical Engineer and Logistics Consultant
U.S. Army DEVCOM Chemical Biological Center

📅 2016–2018 📍 Edgewood, MD

- 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

Chemical Engineer and Logistics Consultant
U.S. Army DEVCOM Chemical Biological Center

📅 2016–2018 📍 Edgewood, MD

- 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 OUTREACH

Department Symposium Co-Chair, Graduate Student
University of Michigan

📅 2019–2024 📍 Ann Arbor, MI

- Served as a co-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.

Volunteer Science Fair Judge
U.S. Army Edgewood Chemical Biological Center

📅 2017 📍 Cecil County, MD

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

TEACHING EXPERIENCE

Graduate Student Instructor
University of Michigan

📅 2019–2021   📍 Ann Arbor, MI

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 44 students to teach a data science course with an emphasis on machine learning. Facilitated laboratory exercises for 2 sections of 22 students each, held weekly office hours, and graded homework assignments.
- Created a Python framework to automate grading group assignments, including rapid data entry via Google Forms and integration with Canvas LMS, shortening our grading time from a week to just 3 days.

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 semiweekly office hours, and conducted 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. Developed a laboratory assignment and held office hours to help students practice basic machine learning.

Administrative Teaching Assistant
Cornell University

📅 2013, 2016   📍 Ithaca, NY

ChemE 3320 – Analysis of Separation Processes (Fall 2017):
- Conducted a complete LaTeX rewrite of a 140-page course textbook, including over 160 figures and 330 equations, for student audiences of 40–70 students. The revised edition received positive feedback from instructors and students.

PUBLICATIONS

- <u>Samuel D. Young</u>. Exploring deep-learning and equivariant machine-learning models for molecular dynamics of aqueous Li–Mn–Cl battery electrolytes. *Technical report* (U.S. Army DEVCOM Army Research Laboratory) **2025**. Adelphi, MD, United States. https://samueldy.github.io/publication/ml-md-limncl-electrolytes.

- <u>Samuel D. Young</u>, 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.

- <u>Samuel D. Young</u>, 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, <u>Samuel D. Young</u>, 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.

- <u>Samuel D. Young</u>, 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, <u>Samuel D. Young</u>, 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, <u>Samuel D. Young</u>, John A. Marohn, *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 D. Young</u>. "Heterogeneous Electrocatalysts for Aqueous Nitrate Reduction and Nitrogen Chemistry". U.S. Army DEVCOM Research Lab Distinguished Postdoctoral Fellowship Candidate Seminar, 12 Oct 2023. Virtual. *Invited seminar as a Distinguished Postdoctoral Fellowship finalist.*

- <u>Samuel D. Young</u>, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. "Thermodynamic Stability and Anion Ordering in ABO_2N and $ABON_2$ Perovskite Oxynitrides". 44th Annual Symposium of the Michigan Chapter of the North American Catalysis Society, 16 May 2023. Ann Arbor, MI, United States.

- <u>Samuel D. Young</u>, Amitava Banerjee, Bryan Goldsmith, Ghanshyam Pilania. "Thermodynamic Stability and Anion Ordering in ABO_2N and $ABON_2$ Perovskite Oxynitrides". 2022 AIChE Annual Meeting, 18 Nov 2022. Phoenix, AZ, United States.

- <u>Samuel D. Young</u>, 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.

- <u>Samuel D. Young</u>, 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.*

- <u>Samuel D. Young</u>, 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, <u>Samuel D. Young</u>, Nirala Singh, Bryan Goldsmith. "Platinum-Ruthenium Alloys As Electrocatalysts for Efficient Aqueous Nitrate Reduction". 2021 AIChE Annual Meeting, 16 Nov 2021. Virtual.

- Danielle Richards, <u>Samuel D. Young</u>, Nirala Singh, Bryan Goldsmith. "Rhodium Sulfide Electrocatalysts for Electrocatalytic Nitrate Reduction". ACS Fall 2021 Meeting, 26 August 2021. Virtual.

- Zixuan Wang, <u>Samuel D. Young</u>, Nirala Singh, Bryan Goldsmith. "Platinum-Ruthenium Alloys as Electrocatalysts for Efficient Aqueous Nitrate Reduction". ACS Spring 2021 Meeting, 13 April 2021. Virtual.

- <u>Samuel D. 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), August 2019. University of Barcelona, Barcelona, Spain.

- <u>Samuel D. Young</u>, Ryan Dwyer, John Marohn. "Interferometric Measurement of Thin-Film Corrosion in Fuel Cell Materials" (poster). Cornell University, April 2016. Ithaca, NY, United States.