

Kevin P. Greenman

 kgreenman@catholic.tech  orcid.org/0000-0002-6466-1401
 kevinsgreenman.com  linkedin.com/in/kevinsgreenman

ACADEMIC POSITION

Catholic Institute of Technology <i>Assistant Professor, Chemistry + Chemical Engineering</i>	Castel Gandolfo, Italy <i>August 2024 – Present</i>
---	--

EDUCATION

Massachusetts Institute of Technology <i>Ph.D. in Chemical Engineering and Computation</i>	Cambridge, MA, USA <i>September 2019 – May 2024</i>
<ul style="list-style-type: none">Advisors: Rafael Gómez-Bombarelli & William H. GreenThesis: “Optical Property Prediction and Molecular Discovery through Multi-Fidelity Deep Learning and Computational Chemistry”Selected Elective Coursework: Numerical Methods in Chemical Engineering; Quantum Chemical Simulation; Parallel Computing and Scientific Machine Learning; Introduction to Quantum Computing; Machine Learning for Molecular Engineering; Process Data Analytics	
University of Michigan <i>B.S.E. in Chemical Engineering (Summa Cum Laude)</i>	Ann Arbor, MI, USA <i>September 2015 – May 2019</i>
<ul style="list-style-type: none">Minor: MathematicsConcentration: Materials Science and EngineeringEngineering Honors Program (Focus: Research)Selected Elective Coursework: Applied Data Science for Engineers; Numerical Methods; Structures of Materials; Electrical/Magnetic/Optical Materials; Physics of Materials; Boundary Value Problems in PDEs	
Hong Kong University of Science and Technology <i>International Summer Exchange Program</i>	Kowloon, Hong Kong <i>June 2016 – August 2016</i>

PAST PROFESSIONAL AND RESEARCH POSITIONS

Massachusetts Institute of Technology <i>NSF Graduate Research Fellow / Graduate Research Assistant</i>	Cambridge, MA, USA <i>January 2020 – May 2024</i>
<ul style="list-style-type: none">Integrated machine learning with physics-based calculations and collaborate with experimental colleagues to predict molecular optical properties using multi-fidelity methodsImplemented uncertainty quantification & active learning to acquire data for model improvementUtilized generative models to propose molecules that satisfy multi-objective constraints	
Eli Lilly and Company <i>Medicines Innovation Hub Intern</i>	Indianapolis, IN, USA <i>May 2022 – August 2022</i>
<ul style="list-style-type: none">Implemented predictive modeling and active learning for imbalanced biological assay dataEvaluated quality of impurity predictions in ASKCOS software	
Microsoft Research New England <i>Micro-intern (Mentors: Kevin K. Yang & Ava P. Amini)</i>	Cambridge, MA, USA <i>January 2022</i>
<ul style="list-style-type: none">Implemented a panel of machine learning uncertainty quantification methods and metrics to benchmark performance on protein engineering tasks with varied domain shifts	
University of Michigan <i>Undergraduate Researcher (Prof. Emmanouil Kioupakis Group)</i>	Ann Arbor, MI, USA <i>September 2017 – May 2019</i>
<ul style="list-style-type: none">Performed first-principles density functional theory calculations using VASP to calculate structural, electronic, and thermodynamic properties of nitride semiconductors	

- Demonstrated quaternary alloy strategy to mitigate lattice mismatch and increase efficiency of InGaN LED materials

Undergraduate Researcher (Prof. Katsuyo Thornton Group)

June 2017 – August 2017

- Simulated lithiation/delithiation processes for core-shell cathode nanoparticles in Li-ion batteries
- Proposed an effective solution to capacity reduction observed in certain nanoparticle designs

Undergraduate Researcher (Prof. Max Shtein Group)

September 2016 – May 2017

- Created a novel type of spring and characterized its mechanical properties
- Designed a testing plan and apparatus to measure stress-strain behavior of kirigami cut patterns

Purdue University

West Lafayette, IN, USA

Summer Undergraduate Research Fellow (Prof. Peilin Liao Group)

May 2018 – August 2018

- **Network for Computational Nanotechnology:** Developed an open-source tool for nanoHUB.org using Quantum ESPRESSO, Python, and the Atomic Simulation Environment (ASE) to calculate properties of interest for heterogeneous catalysis from first principles

Battle Creek Municipal Wastewater Treatment Plant

Battle Creek, MI, USA

Laboratory Intern

January 2015 – May 2015

- Conducted laboratory tests to evaluate water treatment efficacy
- Monitored pollutant levels in industrial effluent

PUBLICATIONS

([Google Scholar](#) | [ResearchGate](#))

(*) denotes equal contribution; (†) denotes corresponding author

Peer-Reviewed Journal Papers

12. David E. Graff, Nathan K. Morgan, Jackson W. Burns, Anna C. Doner, Brian Li, Shih-Cheng Li, Joel Manu, Angiras Menon, Hao-Wei Pang, Haoyang Wu, Akshat Shirish Zalte, Jonathan W. Zheng, Connor W. Coley, William H. Green[†], **Kevin P. Greenman**[†]. “Chemprop v2: An Efficient, Modular Machine Learning Package for Chemical Property Prediction”. Accepted in *Journal of Chemical Information and Modeling* (2025). DOI: [10.26434/chemrxiv-2025-4p1nr](https://doi.org/10.26434/chemrxiv-2025-4p1nr).
11. Nofit Segal, Aviv Netanyahu, **Kevin P. Greenman**, Pulkit Agrawal, Rafael Gómez-Bombarelli. “Known Unknowns: Out-of-Distribution Property Prediction in Materials and Molecules”. *npj Computational Materials*, 11(1), 345 (2025). DOI: [10.1038/s41524-025-01808-x](https://doi.org/10.1038/s41524-025-01808-x).
10. Yizhe Chen*, Shomik Verma*, **Kevin P. Greenman***, Haoyu Yin, Zhihao Wang, Lanjing Wang, Jiali Li, Rafael Gómez-Bombarelli, Aron Walsh, Xiaonan Wang, “A unified active learning framework for photosensitizer design”. *Chemical Science*, (2025). DOI: [10.1039/D5SC05749C](https://doi.org/10.1039/D5SC05749C).
9. Akshay Subramanian, James Damewood, Juno Nam, **Kevin P. Greenman**, Avni P. Singhal, Rafael Gómez-Bombarelli. “Symmetry-constrained generation of diverse low-bandgap molecules with Monte Carlo tree search”. *Chemical Science*, 16, 10503-10511 (2025). DOI: [10.1039/D4SC08675A](https://doi.org/10.1039/D4SC08675A).
8. **Kevin P. Greenman**, Ava P. Amini, Kevin K. Yang. “Benchmarking uncertainty quantification for protein engineering”. *PLOS Computational Biology*, 21(1), e1012639 (2025). DOI: [10.1371/journal.pcbi.1012639](https://doi.org/10.1371/journal.pcbi.1012639).
7. Esther Heid, **Kevin P. Greenman**, Yunsie Chung, Shih-Cheng Li, David E. Graff, Florence H. Vermeire, Haoyang Wu, William H. Green, Charles J. McGill. “Chemprop: A Machine Learning Package for Chemical Property Prediction”. *Journal of Chemical Information and Modeling*, 64(1), 9–17 (2024). DOI: [10.1021/acs.jcim.3c01250](https://doi.org/10.1021/acs.jcim.3c01250).
6. Brent A. Koscher*, Richard B. Canty*, Matthew A. McDonald*, **Kevin P. Greenman**, Charles J. McGill, Camille L. Bilodeau, Wengong Jin, Haoyang Wu, Florence H. Vermeire, Brooke Jin, Travis Hart, Timothy Kulesza, Shih-Cheng Li, Tommi S. Jaakola, Regina Barzilay, Rafael Gómez-Bombarelli, William H. Green, Klavs F. Jensen. “Autonomous, multiproperty-driven molecular discovery: from predictions to measurements and back”. *Science*, 382(6677), eadi1407 (2023). DOI: [10.1126/science.adl1407](https://doi.org/10.1126/science.adl1407).

5. Akshay Subramanian*, **Kevin P. Greenman***, Alexis Gervaix, Tzuhsiu Yang, Rafael Gómez-Bombarelli. “Automated patent extraction powers generative modeling in focused chemical spaces”. *Digital Discovery*, 2(4), 1006–1015 (2023). DOI: [10.1039/D3DD00041A](https://doi.org/10.1039/D3DD00041A).
4. Simon Axelrod, Daniel Schwalbe-Koda, Somesh Mohapatra, James Damewood, **Kevin P. Greenman**, Rafael Gómez-Bombarelli. “Learning Matter: Materials Design with Machine Learning and Atomistic Simulations”. *Accounts of Materials Research*, 3(3), 343–357 (2022). DOI: [10.1021/accountsmr.1c00238](https://doi.org/10.1021/accountsmr.1c00238).
3. **Kevin P. Greenman**, William H. Green, Rafael Gómez-Bombarelli. “Multi-fidelity prediction of molecular optical peaks with deep learning”. *Chemical Science*, 13(4), 1152–1162 (2022). DOI: [10.1039/D1SC05677H](https://doi.org/10.1039/D1SC05677H).
2. Salwan Butrus, **Kevin Greenman**, Eshita Khera, Irina Kopyeva, Akira Nishii. “An Undergraduate-Led, Research-Based Course that Complements a Traditional Chemical Engineering Curriculum”. *Chemical Engineering Education*, 54(2) (2020).
1. **Kevin Greenman**, Logan Williams, Emmanouil Kioupakis. “Lattice-constant and band-gap tuning in wurtzite and zincblende BInGaN alloys”. *Journal of Applied Physics*, 126(055702) (2019). DOI: [10.1063/1.5108731](https://doi.org/10.1063/1.5108731).

Conference Workshop Papers

3. Nofit Segal, Aviv Netanyahu, **Kevin P. Greenman**, Pulkit Agrawal, Rafael Gómez-Bombarelli. “Known Unknowns: Out-of-Distribution Property Prediction in Materials and Molecules”. *NeurIPS AI4Mat Workshop 2024 (Spotlight)*.
2. Akshay Subramanian, James Damewood, Juno Nam, **Kevin P. Greenman**, Avni P. Singhal, Rafael Gómez-Bombarelli. “Symmetry-Constrained Generation of Diverse Low-Bandgap Molecules with Monte Carlo Tree Search”. *NeurIPS AI4Mat Workshop 2024*.
1. **Kevin P. Greenman**, Ava P. Amini, Kevin K. Yang. “Benchmarking Uncertainty Quantification for Protein Engineering”. *ICLR Machine Learning for Drug Discovery (MLDD) Workshop 2022*.

In Preparation

2. **Kevin P. Greenman**, Temujin Orkhon, William H. Green, Rafael Gómez-Bombarelli. “Multi-Fidelity Deep Learning for Data-Efficient Molecular Property Models from Experimental and Computational Data”. (In preparation).
1. **Kevin P. Greenman**, Rui-Xi Wang, Juno Nam, Akshay Subramanian, Jurgis Ruza, Joonyoung F. Joung, Minhi Han, William H. Green, Sungnam Park, Rafael Gómez-Bombarelli. “Benchmarking predictions of near-infrared absorption with physics-based and machine learning methods”. (In preparation).

Other

2. **Kevin Greenman**, Peilin Liao. “Computational Catalysis: Creating a User-Friendly Tool for Research and Education”. The Summer Undergraduate Research Fellowship Symposium (2018). Paper 129.
1. **Kevin Greenman**, Peilin Liao. “Computational Catalysis with Density Functional Theory”. *nanoHUB* resource (2018). DOI: [10.4231/D3PK0743B](https://doi.org/10.4231/D3PK0743B).

SELECTED OPEN-SOURCE SOFTWARE CONTRIBUTIONS

([GitHub](#) | [nanoHUB](#))

- **Chemprop** – Co-Maintainer (2021–2024). Open-source package for chemical property prediction. 2,000+ GitHub stars. 1.4MM+ PyPI downloads. <https://github.com/chemprop/chemprop>
- Kevin Greenman. “Chemprop Demo” (2022). *nanoHUB* resource. DOI: [10.21981/ZPYJ-CF14](https://doi.org/10.21981/ZPYJ-CF14).
- Kevin Greenman, Peilin Liao. “Computational Catalysis with DFT” (2018). *nanoHUB* resource. DOI: [10.4231/D3PK0743B](https://doi.org/10.4231/D3PK0743B).

PRESENTATIONS

Invited Talks

7. **Kevin P. Greenman.** “Artificial Intelligence and Physics-Based Simulations for (Bio)Molecular and Materials Design”. *Physics Department, University of Rome Tor Vergata* (Rome, Italy) (November 2025).
6. **Kevin P. Greenman.** “Optical Property Prediction and Molecular Discovery through Multi-Fidelity Deep Learning and Computational Chemistry”. *MIT Signals Information and Algorithms (Prof. Gregory Wornell) Group Meeting* (Virtual) (September 2025).
5. **Kevin P. Greenman.** “AI-driven chemistry research and undergraduate skill development with Chemprop”. *ACS Fall Meeting*, Washington, D.C., USA (August 2025).
4. **Kevin P. Greenman.** “Chemprop and Related Projects”. *Axiom Bio Journal Club* (Virtual) (May 2025).
3. **Kevin P. Greenman.** “Multi-fidelity deep learning for data-efficient molecular property models from experimental and computational data”. *MIT Machine Learning in Biology Working Group*, Cambridge, MA, USA (May 2024).
2. **Kevin P. Greenman.** “Message-Passing Neural Networks for Molecular Property Prediction Using Chemprop”. *nanoHUB Hands-on Data Science and Machine Learning Training Series* (Virtual) (April 2022). [[nanoHUB](#) | [YouTube](#)]
1. **Kevin P. Greenman.** “Fast, Accurate, and Generalizable Prediction of Molecular Optical Properties from Multi-fidelity Data”. *ARPA-E DIFFERENTIATE Meeting*, Carnegie Mellon University (Virtual) (March 2022).

Contributed Talks

11. **Kevin P. Greenman**, Rui-Xi Wang, Joonyoung F. Joung, Minhi Han, William H. Green, Sungnam Park, Rafael Gómez-Bombarelli. “Toward Accurate Prediction of Near-Infrared Absorption: Physics-Based Calculations, Machine Learning, and the Crucial Role of Data”. *AICHE Annual Meeting*, Boston, MA, USA (November 2025).
10. **Kevin P. Greenman**, Temujin Orkhon, William H. Green, Rafael Gómez-Bombarelli. “Data-Driven Strategy Selection for Multi-Fidelity Modeling in Autonomous Molecular Discovery”. *AICHE Annual Meeting*, Boston, MA, USA (November 2025).
9. **Kevin P. Greenman**. “Harnessing AI for Scientific Discovery: Achievements, Opportunities, and Ethical Reflections”. *Society of Catholic Scientists Conference*. Mundelein, IL, USA (June 2024). [[YouTube](#)]
8. **Kevin Greenman**. “Chemprop v1.7.1 & v2.0.0: Stable Release and Benchmarks”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*. Cambridge, MA, USA (April 2024).
7. **Kevin Greenman**. “Chemprop v2.0.0: New Features and Updates”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*. Cambridge, MA, USA (October 2023).
6. **Kevin P. Greenman**, Akshay Subramanian, Alexis Gervaix, Rafael Gómez-Bombarelli. “Automatic chemical dataset generation, labeling, and modeling from patent literature queries”. *ACS Fall Meeting*, Chicago, IL, USA (August 2022).
5. **Kevin P. Greenman**, William H. Green, Rafael Gómez-Bombarelli. “Multi-Fidelity Deep Learning and Active Learning for Molecular Optical Properties”. *International Symposium on Molecular Spectroscopy*, Urbana, IL, USA (June 2022).
4. **Kevin P. Greenman**, William H. Green, Rafael Gómez-Bombarelli. “Transfer Learning for Prediction of Absorption and Emission Spectra from Multi-fidelity Data”. *AICHE Annual Meeting*, Boston, MA, USA (November 2021).
3. **Kevin P. Greenman**, Simon Axelrod, William H. Green, Rafael Gómez-Bombarelli. “Predicting absorption spectra of molecular dyes using deep learning”. *ACS Spring Meeting* (Virtual) (April 2021).

2. **Kevin Greenman**, Logan Williams, Emmanouil Kioupakis. “Lattice Constant and Band Gap Tuning in BInGaN Alloys for Next-Generation LEDs”. *APS March Meeting*, Boston, MA, USA (March 2019).
1. **Kevin Greenman**. “Computational Catalysis – Creating a User-Friendly Tool for Research and Education”. *nanoHUB 3-minute Research Talk*, West Lafayette, IN, USA (August 2018).

Workshops / Workshop Talks

3. Gergely Gidofalvi, **Kevin Greenman**, Prajay Patel, Dominic Sirianni, Marie van Staveren, Cecilia Vollbrecht. “Get Programming into Your Course: Free Online Teaching Modules for Chemistry Courses”. *Biennial Conference on Chemical Education (BCCE) 2026*. Madison, WI, USA (Accepted).
2. **Kevin P. Greenman**, Haoyang Wu, William H. Green. “Chemprop: Datasets and Machine Learning Software for Chemical Property Prediction”. Division of Catalysis Science and Technology (CATL) – Open Source Software Workshops, *ACS Fall Meeting*. San Francisco, CA, USA (August 2023).
1. Charles McGill, Michael Forsuelo, **Kevin P. Greenman**. “An Introduction to Chemprop”. *Enko (Virtual)* (February 2022).

Posters

13. David E. Graff, **Kevin P. Greenman**, Hao-Wei Pang, Nathan Morgan, Jackson Burns, Angiras Menon, Shih-Cheng Li, Haoyang Wu, Jonathan Zheng, Anna Doner, Xiaorui Dong, Joel Manu, Kevin Spiekermann, William H. Green. “Chemprop v2.0.0: Stable Release and Future Plans”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*, Cambridge, MA, USA (April 2024).
12. **Kevin P. Greenman**, Temujin Orkhon, William H. Green, Rafael Gómez-Bombarelli. “Multi-Fidelity Deep Learning for Data-Efficient Molecular Property Models from Experimental and Computational Data”. *AICHE Annual Meeting*, Orlando, FL, USA (November 2023).
11. **Kevin P. Greenman**. “Multi-Fidelity Computer-Aided Molecular Design”. *AICHE Annual Meeting*, Orlando, FL, USA (November 2023).
10. **Kevin P. Greenman**, Temujin Orkhon, William H. Green, Rafael Gómez-Bombarelli. “Multi-Fidelity Deep Learning for Data-Efficient Molecular Property Models from Experimental and Computational Data”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*, Cambridge, MA, USA (October 2023).
9. David Graff, **Kevin P. Greenman**, Nathan Morgan, Oscar Wu, Angiras Menon, Hao-Wei Pang, Xiaorui Dong, Jackson Burns, Kevin Spiekermann, William H. Green. “Chemprop New Features and Updates”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*, Cambridge, MA, USA (October 2023).
8. **Kevin P. Greenman**, Ava P. Amini, Kevin K. Yang. “Benchmarking Uncertainty Quantification for Protein Engineering”. *ACS Fall Meeting*, San Francisco, CA, USA (August 2023).
7. David Graff, **Kevin P. Greenman**, Oscar Wu, Shih-Cheng Li, and William H. Green. “Chemprop New Upcoming Features and Updates”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*, Cambridge, MA, USA (May 2023).
6. **Kevin P. Greenman**, Ava P. Soleimany, and Kevin K. Yang. “Benchmarking Uncertainty Quantification for Protein Engineering”. *International Conference on Learning Representations – Machine Learning for Drug Discovery Workshop*, Virtual (April 2022).
5. David Graff, **Kevin P. Greenman**, Oscar Wu, Shih-Cheng Li, William H. Green. “Chemprop v1.5.0 New Features and Updates”. *Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting*, Cambridge, MA, USA (April 2022).
4. **Kevin P. Greenman**, William H. Green, Rafael Gómez-Bombarelli. “Artificial Intelligence Applications in the Design of Novel Dye Molecules with Targeted Optical Properties”. *Society of Catholic Scientists Conference*, Washington, DC, USA (June 2021).

3. **Kevin Greenman**, Logan Williams, Emmanouil Kioupakis. "Lattice-Constant and Band-Gap Tuning in BInGaN Alloys for Higher-Efficiency LEDs". *University of Michigan Engineering Design Expo*, Ann Arbor, MI, USA (April 2019).
2. **Kevin Greenman**, Peilin Liao. "Computational Catalysis with Density Functional Theory". *AICHE Undergraduate Student Poster Competition*, Pittsburgh, PA, USA (October 2018).
1. **Kevin Greenman**, Peilin Liao. "Computational Catalysis with Density Functional Theory". *Network for Computational Nanotechnology Undergraduate Research Experience Poster Session*, West Lafayette, IN, USA (July 2018).

TEACHING EXPERIENCE & PEDAGOGICAL TRAINING

Catholic Institute of Technology	Castel Gandolfo, Italy
<i>Instructor</i>	<i>August 2024 – Present</i>
<ul style="list-style-type: none"> • General Chemistry (Fall 2025) - <i>planned from scratch</i> • Seminar in Research + Engineering Practice (Fall 2024, Winter 2025, Spring 2025, Fall 2025) • Differential + Integral Calculus (Fall 2024) - <i>planned from scratch</i> 	
Massachusetts Institute of Technology	Cambridge, MA, USA
<i>Guest Lecturer: Introduction to Modeling and Simulation</i>	<i>April 2024</i>
<ul style="list-style-type: none"> • Lecture on density functional theory for undergraduates 	
<i>Graduate Teaching Assistant: Machine Learning for Molecular Engineering</i>	<i>January 2022 – May 2022</i>
<ul style="list-style-type: none"> • Faculty: Profs. Connor Coley, Ernest Fraenkel, Rafael Gómez-Bombarelli • Coordinated with faculty and one TA to prepare/grade assignments, hold weekly office hours, and manage course logistics for 60 students (undergraduate & graduate) 	
MIT Teaching + Learning Lab	Cambridge, MA, USA
<i>TA Days Training</i>	<i>January 2022</i>
<ul style="list-style-type: none"> • Learned strategies to support student well-being and to facilitate effective office hours 	
<i>Grad Teaching Development Tracks Certificate Program</i>	<i>June 2020 – May 2021</i>
<ul style="list-style-type: none"> • Inclusive Teaching Track (May 2021); Microteaching Track (March 2021); Lesson Planning Track (January 2021); Subject Design Track (June 2020) 	
MIT Chemical Engineering Teach-Off Competition	Cambridge, MA, USA
<i>1st Place Awardee</i>	<i>April 2021</i>
<ul style="list-style-type: none"> • Prepared and taught a 10-minute virtual lesson and was judged to be the best out of seven graduate student and postdoc competitors in the department by a panel of teaching experts 	
University of Michigan Department of Chemical Engineering	Ann Arbor, MI, USA
<i>Computational Lead – Chemical Engineering Team – Perch Education</i>	<i>February 2018 – May 2019</i>
<ul style="list-style-type: none"> • Created the computational curriculum for a new class to reduce barriers to undergraduate research in collaboration with faculty, graduate students, and undergraduate students 	
<i>Instructional Aide – Fluid Mechanics</i>	<i>January – April 2018, January – April 2019</i>
<ul style="list-style-type: none"> • Coordinated with one other instructional aide to prepare practice problems, teach a weekly review session, and hold weekly office hours for 100 students 	
University of Michigan Science Learning Center	Ann Arbor, MI, USA
<i>Study Group Facilitator – Organic Chemistry II – 2 semesters</i>	<i>January – December 2017</i>
<ul style="list-style-type: none"> • Facilitated a two-hour weekly study session to help thirteen group members improve understanding of material • Attended workshops on evidence-based teaching and learning techniques 	

MENTORSHIP

CatholicTech Undergraduate Students

2. Mary Holler (Summer 2025) - *Capstone Project*
1. Lauren Mitchell (Summer 2025) - *Research Thesis Project*

MIT Professional Development Certificate in Research Mentoring (January 2024)

MIT Undergraduate Research Opportunity Program (UROP)

6. Joel Manu (IAP 2024, Spring 2024, Summer 2024)
5. Temujin Orkhon (Spring 2023, Fall 2023, Spring 2024) - *1st place MIT ChemE UROP poster session (April 2024)*
4. Rui-Xi (Ray) Wang (Spring 2023, Fall 2023, Spring 2024)
3. Alor Sahoo (Fall 2022)
2. Cale Gregory (Spring 2022)
1. Eleenna Kim (Spring 2022)

OUTREACH

MIT ChemE Application Mentorship Program (ChAMP)	Fall 2020, 2021
MIT Netpals	January – May 2020
MIT Graduate Application Assistance Program (GAAP)	Fall 2019

HONORS & AWARDS

LLM Hackathon for Applications in Materials Science & Chemistry Lila Prize (September 2025) - 3rd place out of 120 teams in global 2-day hackathon competition, and 2nd place among MIT teams.

MolSSI ACT-CMS Faculty Fellowship (2024-2026) - 1 of 10 inaugural fellows selected for curriculum development program that facilitates the integration of programming, computation, and other cyberinfrastructure skills into existing molecular science courses.

National Science Foundation Graduate Research Fellowship (2021-2024) – Tuition and stipend for 3 years of graduate study and research.

Tau Beta Pi Fellowship (2020) – Awarded by the Tau Beta Pi Association to 30 students in the nation on the basis of scholarship, leadership and service, and the promise of substantial achievement.

Robert T. Haslam (1911) MIT Chemical Engineering Fellowship (2019) - Full tuition and stipend for one academic year.

Dean's List (2015-2019) – Awarded by the University of Michigan College of Engineering for 8 consecutive semesters.

Henry Ford II Prize (2018) – Awarded to the top junior in the University of Michigan College of Engineering.

Tau Beta Pi Scholarship (2018) – Awarded by the Tau Beta Pi Association on the basis of academic achievement, extracurricular activities, and the promise of substantial contributions to the engineering profession.

Chevron Scholarship (2017) - University of Michigan College of Engineering

Jane and Howard TenBroeck Scholarship (2017) - University of Michigan Chemical Engineering

AIChE Donald F. Othmer Sophomore Academic Excellence Award (2017) – Presented to one AIChE student member in each student chapter who has attained the highest scholastic grade-point average during his/her freshman and sophomore years, on recommendation of the Student Chapter Advisor.

A.H. White Scholarship (2017) - University of Michigan Chemical Engineering

Julius F. Bartus Endowed Memorial Scholarship (2016-2019) - University of Michigan College of Engineering

Tau Beta Pi First-Year Award (2016) – Awarded by the Michigan Gamma chapter to three first-year students in the College of Engineering.

William J. Branstrom Freshman Prize (2016) – Awarded by the University of Michigan for ranking in the top 5% of the College of Engineering freshman class after the first term.

Regents Merit Scholarship (2015) - University of Michigan

PROFESSIONAL AFFILIATIONS

American Society of Engineering Education (ASEE)	July 2023 – Present
U.S. Research Software Engineer Association (US-RSE)	March 2023 – Present
American Chemical Society (ACS)	March 2021 – Present
Society of Catholic Scientists	May 2019 – Present
<i>Harvard-MIT Chapter Co-Founder and Co-President</i>	<i>August 2022 – August 2024</i>
Tau Beta Pi Engineering Honor Society	December 2016 – Present
<i>MI-G Chapter Advisor</i>	<i>January – April 2019</i>
<i>MI-G Chapter President</i>	<i>April – December 2018</i>
• Managed a team of 17 officers and 7 advisors to carry out chapter programming/operations	
• Engaged ~200 members in service, social, and professional development events	
<i>MI-G Chapter Professional Development Officer</i>	<i>April 2017 – April 2018</i>
• Planned and promoted 17 corporate info sessions on campus for up to 150 attendees	
American Institute of Chemical Engineers (AIChE)	September 2016 – Present
Materials Research Society (MRS)	2024 – 2025
American Physical Society (APS)	2018 – 2019

TECHNICAL SKILLS

Languages: Python | shell (bash/zsh) | MATLAB | Julia | Mathematica | C++ | Fortran

Tools: RDKit | git | vim | LaTeX | Django | Drupal | Wordpress

Software: PyTorch | ORCA | VASP | Quantum Espresso | Avogadro | VESTA | ChemDraw | Aspen Plus | COMSOL Multiphysics | SolidWorks

Project Management: Agile | Kanban | Scrum

Platforms: Mac | Linux | Windows

PROFESSIONAL SERVICE

Awesome Chemical Engineering Education

Creator and Maintainer

June 2023 – Present

- Curate an open-source list of online chemical engineering education resources
- <https://github.com/kevingreenman/awesome-chemical-engineering-education>

Scientific Service

Editorial

- *Journal of Responsible Technology* - Associate Editor (2025 – Present)

Journal Peer Review

- *Communications Chemistry*
- *Digital Discovery* (data reviewer)
- *Scientific Data*

Conference/Workshop Peer Reviewer

- NeurIPS Machine Learning and the Physical Sciences (MLPS) workshop (2025)
- NeurIPS AI for Accelerated Materials Discovery (AI4Mat) workshop (2025)
- ICML Exploration in AI Today (EXAIT) workshop (2025)
- ICLR Generative and Experimental Perspectives (GEM) for BioMolecular Design workshop (2024, 2025)
- Learning on Graphs (LoG) Conference (2022, 2023, 2024, 2025)
- NeurIPS Adaptive Experimental Design and Active Learning in the Real World workshop (2023)

Grant Peer Review

- Dutch Research Council (NWO) Applied and Engineering Sciences (AES) Open Technology Programme (2025)

Catholic Institute of Technology

- Undergraduate Admissions Committee (2024-2025)

MIT Chemical Engineering Department

Graduate Student Council for Course 10 (GSC-X)

July 2020 – August 2021

- Coordinated intramural sports teams and social events to promote community and well-being

Michigan Undergraduate Research Symposium

Co-Founder and Organizer

November 2018 – May 2019

- Raised over \$12,000 in funding to support the first annual symposium for undergraduates from all disciplines to present research on campus and earn travel awards to present at conferences
- Collaborated with six other undergraduates to organize the event with 150 presenters and 100 judges