

# Kevin P. Greenman

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## ACADEMIC POSITION

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

<b>Massachusetts Institute of Technology</b> <i>Ph.D. in Chemical Engineering and Computation</i>	Cambridge, MA, USA <i>September 2019 – May 2024</i>
<ul style="list-style-type: none"><li><b>Advisors:</b> Rafael Gómez-Bombarelli &amp; William H. Green</li><li><b>Thesis:</b> “Optical Property Prediction and Molecular Discovery through Multi-Fidelity Deep Learning and Computational Chemistry”</li><li><b>Selected Elective Coursework:</b> 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</li></ul>	
<b>University of Michigan</b> <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"><li><b>Minor:</b> Mathematics</li><li><b>Concentration:</b> Materials Science and Engineering</li><li>Engineering Honors Program (Focus: Research)</li><li><b>Selected Elective Coursework:</b> Applied Data Science for Engineers; Numerical Methods; Structures of Materials; Electrical/Magnetic/Optical Materials; Physics of Materials; Boundary Value Problems in PDEs</li></ul>	
<b>Hong Kong University of Science and Technology</b> <i>International Summer Exchange Program</i>	Kowloon, Hong Kong <i>June 2016 – August 2016</i>

## PAST PROFESSIONAL AND RESEARCH POSITIONS

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

- 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 Shtain 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

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. Carty\*, 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*.

#### *Preprint / Submitted / Under Review / Accepted*

1. 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”. *chemRxiv*. DOI: [10.26434/chemrxiv-2025-4p1nr](https://doi.org/10.26434/chemrxiv-2025-4p1nr). (Under Revision at *Journal of Chemical Information and Modeling*).

#### *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).

- **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).

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## PRESENTATIONS

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### *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*

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

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

## MENTORSHIP

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### 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. Elenna Kim (Spring 2022)

## OUTREACH

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

## HONORS & AWARDS

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**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

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<b>American Society of Engineering Education (ASEE)</b>	July 2023 – Present
<b>U.S. Research Software Engineer Association (US-RSE)</b>	March 2023 – Present
<b>American Chemical Society (ACS)</b>	March 2021 – Present
<b>Society of Catholic Scientists</b>	May 2019 – Present
<i>Harvard-MIT Chapter Co-Founder and Co-President</i>	<i>August 2022 – August 2024</i>
<b>Tau Beta Pi Engineering Honor Society</b>	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	
<b>American Institute of Chemical Engineers (AIChE)</b>	September 2016 – Present
<b>Materials Research Society (MRS)</b>	2024 – 2025
<b>American Physical Society (APS)</b>	2018 – 2019

## TECHNICAL SKILLS

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**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

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### **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