KEVIN P. GREENMAN

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EDUCATION

Massachusetts Institute of Technology Cambridge, MA

Ph.D. Candidate in Chemical Engineering and Computation September 2019 – Present

- 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

Graduate Certificate in Technical Leadership September 2020 – Present

- Coursework: Negotiation and Influence Skills for Technical Leaders

University of Michigan Ann Arbor, MI

B.S.E. in Chemical Engineering (*Summa Cum Laude*) September 2015 – May 2019

- Concentration in Materials Science and Engineering, Minor in Mathematics
- Engineering Honors Program (Focus Area: Research)
- 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 Kowloon, Hong Kong

International Summer Exchange Program June – August 2016

RESEARCH EXPERIENCE

Massachusetts Institute of Technology

Doctoral Advisors: Rafael Gómez-Bombarelli and William Green (January 2020 – Present)

- Integrate machine learning with physics-based calculations and collaborate with experimental colleagues to predict molecular optical properties using multi-fidelity methods
- Implement uncertainty quantification and active learning to acquire data for model improvement
- Utilize generative models to propose molecules that satisfy multi-objective constraints

Microsoft Research New England (Micro-internship)

Mentors: Kevin K. Yang and Ava P. Soleimany (January 2022)

- 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

Prof. Emmanouil Kioupakis Group (September 2017 – May 2019)

- 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

Prof. Katsuyo Thornton Group (June – 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

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

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Purdue University Summer Undergraduate Research Fellowship

Network for Computational Nanotechnology – Prof. Peilin Liao Group (May – August 2018)

- Developed an open-source tool for nanoHUB.org using Quantum ESPRESSO, Python, and the Atomic Simulation Environment to calculate properties of interest for heterogeneous catalysis from first principles

PUBLICATIONS

(Google Scholar | ResearchGate)

Forthcoming

1. **Kevin P. Greenman**, Ava P. Soleimany, and Kevin K. Yang, "Benchmarking Uncertainty Quantification for Protein Engineering". (In preparation).

Peer-Reviewed Journals

1. Simon Axelrod, Daniel Schwalbe-Koda, Somesh Mohapatra, James Damewood, **Kevin P. Greenman**, and Rafael Gómez-Bombarelli, "Learning Matter: Materials Design with Machine Learning and Atomistic Simulations". Acc. Mater. Res. (2022), 3(3), 343–357. DOI: 10.1021/accountsmr.1c00238.
2. **Kevin P. Greenman**, William H. Green, and Rafael Gómez-Bombarelli, "Multi-fidelity prediction of molecular optical peaks with deep learning". Chemical Science (2022), 13(4), 1152 - 1162. DOI: 10.1039/D1SC05677H.
3. Salwan Butrus, **Kevin Greenman**, Eshita Khera, Irina Kopyeva, and Akira Nishii, "An Undergraduate-Led, Research-Based Course that Complements a Traditional Chemical Engineering Curriculum". Chemical Engineering Education (2020), 54(2).
4. **Kevin Greenman**, Logan Williams, and Emmanouil Kioupakis, "Lattice-constant and band-gap tuning in wurtzite and zincblende BInGaN alloys". J. Appl. Phys. (2019), 126(055702). DOI: 10.1063/1.5108731.

Other

1. **Kevin Greenman** and Peilin Liao (2018), "Computational Catalysis: Creating a User-Friendly Tool for Research and Education". The Summer Undergraduate Research Fellowship (SURF) Symposium. Paper 129.
2. **Kevin Greenman** and Peilin Liao (2018), "Computational Catalysis with Density Functional Theory," https://nanohub.org/resources/28763.

SOFTWARE CONTRIBUTIONS

(GitHub | nanoHUB)

1. Chemprop (2021 – Present): https://github.com/chemprop/chemprop
2. **Kevin Greenman** (2022), "Chemprop Demo," https://nanohub.org/resources/chempropdemo. DOI: 10.21981/ZPYJ-CF14.
3. **Kevin Greenman** and Peilin Liao (2018), "Computational Catalysis with DFT," https://nanohub.org/resources/compcatal. DOI: 10.4231/D3PK0743B.

PRESENTATIONS

Invited Talks

1. **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)

2. **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.
3. Charles McGill, Michael Forsuelo, and **Kevin Greenman**, "An Introduction to Chemprop", Enko (Virtual), February 2022.

Contributed Talks

1. **Kevin P. Greenman**, William H. Green, and Rafael Gómez-Bombarelli. "Multi-Fidelity Deep Learning and Active Learning for Molecular Optical Properties" International Symposium on Molecular Spectroscopy. Urbana, IL, June 2022 (Accepted).
2. **Kevin P. Greenman**, William H. Green, and Rafael Gómez-Bombarelli. "Transfer Learning for Prediction of Absorption and Emission Spectra from Multi-fidelity Data". American Institute of Chemical Engineers Annual Meeting. Boston, MA, November 2021.
3. **Kevin P. Greenman**, Simon Axelrod, William H. Green, and Rafael Gómez-Bombarelli. "Predicting absorption spectra of molecular dyes using deep learning". American Chemical Society Spring Meeting. Virtual, April 2021.
4. **Kevin Greenman**, Logan Williams, and Emmanouil Kioupakis. "Lattice Constant and Band Gap Tuning in BInGaN Alloys for Next-Generation LEDs". American Physical Society March Meeting. Boston, MA, March 2019.
5. **Kevin Greenman**, "Computational Catalysis – Creating a User-Friendly Tool for Research and Education". nanoHUB 3-minute Research Talk. West Lafayette, IN, August 2018. (nanoHUB)
6. **Kevin Greenman** and Peilin Liao. "Computational Catalysis: Creating a User-Friendly Tool for Research and Education". Purdue Summer Undergraduate Research Fellowship (SURF) Symposium. West Lafayette, IN, August 2018.

Posters

1. **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.
2. Charles McGill, **Kevin Greenman**, David Graff, Oscar Wu, and William H. Green. "Chemprop v1.5.0 New Features and Updates". Machine Learning for Pharmaceutical Discovery and Synthesis Consortium Meeting. Cambridge, MA. April 2022.
3. **Kevin P. Greenman**, William H. Green, and Rafael Gómez-Bombarelli. "Artificial Intelligence Applications in the Design of Novel Dye Molecules with Targeted Optical Properties". Society of Catholic Scientists Conference. Washington, DC, June 2021.
4. **Kevin Greenman**, Logan Williams, and Emmanouil Kioupakis. "Lattice-Constant and Band-Gap Tuning in BInGaN Alloys for Higher-Efficiency LEDs". University of Michigan Engineering Design Expo. Ann Arbor, MI, April 2019.
5. **Kevin Greenman** and Peilin Liao. "Computational Catalysis with Density Functional Theory". American Institute of Chemical Engineers Undergraduate Student Poster Competition. Pittsburgh, PA, October 2018.
6. **Kevin Greenman** and Peilin Liao. "Computational Catalysis with Density Functional Theory". Network for Computational Nanotechnology Undergraduate Research Experience Poster Session. West Lafayette, IN, July 2018.

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TEACHING EXPERIENCE AND PEDAGOGICAL TRAINING

MIT Chemical Engineering Department

Graduate Teaching Assistant: Machine Learning for Molecular Engineering (10.C01/10.C51)

- Faculty: Profs. Connor Coley, Ernest Fraenkel, and Rafael Gómez-Bombarelli
- Coordinated with one other TA to prepare and grade homework assignments, hold weekly office hours, and manage all course logistics for 60 students (undergraduate and graduate)

MIT Teaching + Learning Lab

TA Days Training (January 2022)

- Learned strategies to support student well-being and to facilitate effective office hours

Grad Teaching Development Tracks Certificate Program

- 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

1st Place Awardee (April 2021)

- 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

Instructional Aide – Fluid Mechanics (January – April 2018, January – April 2019)

- 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

Study Group Facilitator – Organic Chemistry II – 2 semesters (January – December 2017)

- 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 EXPERIENCE

Undergraduate Research Opportunity Program (UROP)

- Cale Gregory (Spring 2022)
- Elenna Kim (Spring 2022)

Chemical Engineering Application Mentorship Program (ChAMP) (Fall 2020, 2021)

- Provided application feedback to students from underrepresented backgrounds applying to the chemical engineering Ph.D. program at MIT

Netpals (January – May 2020)

- Mentored a student from a local middle school by practicing email etiquette and discussing science

Graduate Application Assistance Program (GAAP) – Office of Graduate Education (Fall 2019)

- Provided application feedback to a student from an underrepresented background applying to a Ph.D. program at the Institute

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OTHER RELEVANT EXPERIENCE

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

Perch Education

Chemical Engineering Team – Computational Lead (February 2018 – May 2019)

- Created the computational curriculum for a new class to reduce barriers to undergraduate research in collaboration with faculty, graduate students, and undergraduate students

Battle Creek Municipal Wastewater Treatment Plant

Laboratory Intern (January – May 2015)

- Conducted laboratory tests to evaluate efficacy of water treatment methods
- Monitored pollutant levels in water discharged from local factories

HONORS AND AWARDS

- National Science Foundation Graduate Research Fellowship (2021) – 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.
- 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.
- 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.

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PROFESSIONAL AFFILIATIONS

American Chemical Society (March 2021 – Present)

Society of Catholic Scientists (May 2019 – Present)

Tau Beta Pi Engineering Honor Society (December 2016 – Present)
MI-G Chapter Advisor (January – April 2019)
MI-G Chapter President (April – December 2018)

- Managed a team of 17 officers and 7 advisors to carry out chapter programming and operations
- Engaged approximately 200 members in service, social, and professional development events

MI-G Chapter Professional Development Officer (April 2017 – April 2018)

- Planned and promoted 17 corporate information sessions on campus for up to 150 attendees

American Institute of Chemical Engineers (September 2016 – Present)

SKILLS

Languages: Python | shell (bash/zsh) |MATLAB | Julia | Mathematica | C++ | Fortran
Tools: git | vim | LaTeX | Django | Drupal
Software: PyTorch | VASP | Quantum Espresso | Avogadro | VESTA | ChemDraw | Aspen Plus | COMSOL Multiphysics | SolidWorks
Project Management: Agile | Kanban | Scrum
Platforms: Mac | Linux

SERVICE

MIT Chemical Engineering Department
Graduate Student Council for Course 10 (GSC-X) (July 2020 – August 2021)

- Coordinated intramural sports teams and planned virtual social events to promote community and well-being during COVID-19 crisis

St. Mary Student Parish
Alternative Spring Break Site Leader and Participant (2016 – 2018)

- Flint, Michigan (2018 - Site Leader)
- Meridian, Mississippi (2017 - Participant)
- Flint, Michigan (2016 - Participant)

Ig.nite Lead Team Member (2015 – 2017)

- Led effort to convert weekly dinner/speaker event for 150-200 people to zero-waste through composting.

St. Philip Catholic Central High School
Assistant Track & Field Coach (2016 – 2017)

- Coached six high jumpers to new personal bests, and one to be regional champion and all-state.
- Wrote a Python program based on input from other coaches to pre-score track meets.