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

Graduate Certificate in Technical Leadership September 2020 – Present

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

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

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

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PUBLICATIONS

(Google Scholar | ResearchGate)

Journal

1. **Kevin P. Greenman**, William H. Green, and Rafael Gómez-Bombarelli, "Deep learning for absorption peak locations using optimized molecular representations and on-the-fly TD-DFT regularization". (Manuscript in preparation).
2. 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 54, 2 (2020).
3. **Kevin Greenman**, Logan Williams, and Emmanouil Kioupakis, "Lattice-constant and band-gap tuning in wurtzite and zincblende BInGaN alloys". J. Appl. Phys. 126, 055702 (2019); doi: 10.1063/1.5108731.

Other

1. **Kevin Greenman** and Peilin Liao (2018), "Computational Catalysis with DFT," https://nanohub.org/resources/compcatal. doi: 10.4231/D3PK0743B.
2. **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.
3. **Kevin Greenman** and Peilin Liao (2018), "Computational Catalysis with Density Functional Theory," https://nanohub.org/resources/28763.

PRESENTATIONS

Oral Presentations

1. **Kevin P. Greenman**, William H. Green, 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 (Accepted).
2. **Kevin P. Greenman**, Simon Axelrod, William H. Green, Rafael Gómez-Bombarelli. "Predicting absorption spectra of molecular dyes using deep learning". American Chemical Society Spring Meeting. Virtual, April 2021.
3. **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.
4. **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.

Poster Presentations

1. **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, June 2021.
2. **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.
3. **Kevin Greenman** and Peilin Liao. "Computational Catalysis with Density Functional Theory". American Institute of Chemical Engineers Undergraduate Student Poster Competition. Pittsburgh, PA, October 2018.

4. **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.

PRESENTATIONS (CONTRIBUTED)

Oral Presentations

1. Camille Bilodeau, Brent Koscher, **Kevin P. Greenman**, Rafael Gómez-Bombarelli, and Klavs F. Jensen. "Designing and Synthesizing Novel Dye Molecules Using Generative Modeling and Data-Driven Synthesis Planning". American Institute of Chemical Engineers Annual Meeting. Boston, MA, November 2021 (Accepted).
2. Logan Williams, **Kevin Greenman**, and Emmanouil Kioupakis. "First principles calculations of boron alloyed group III nitrides for higher efficiency UV and visible LEDs". 13th International Conference on Nitride Semiconductors. Bellevue, WA, July 2019.
3. Logan Williams, **Kevin Greenman**, and Emmanouil Kioupakis. "First principles calculations of boron alloyed group III nitrides for higher efficiency UV and visible LEDs". 61st Electronic Materials Conference. Ann Arbor, MI, June 2019.
4. Logan Williams, **Kevin Greenman**, and Emmanouil Kioupakis. "Alloying boron into InGaN active layers to create higher-power, higher-efficiency LEDs". University of Michigan Engineering Graduate Symposium 2018 Towner Prize Session. Ann Arbor, MI, November 2018.
5. Logan Williams, **Kevin Greenman**, and Emmanouil Kioupakis. "BInGaN alloys lattice-matched to GaN for high-power high-efficiency visible LEDs". American Physical Society March Meeting. Los Angeles, CA, March 2018.

Poster Presentations

1. Logan Williams, **Kevin Greenman**, and Emmanouil Kioupakis. "Alloying boron into InGaN active layers to create higher-power, higher-efficiency LEDs". University of Michigan MSE Graduate Symposium. Ann Arbor, MI, November 2018.

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
Platforms: Mac | Linux

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TEACHING EXPERIENCE AND PEDAGOGICAL TRAINING

MIT Chemical Engineering Teach-Off 2021

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

MIT Teaching + Learning Lab

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)

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 over 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

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

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

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

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)

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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.
- 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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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.