When I began my undergraduate studies at the University of Michigan (U-M), the thought of pursuing a Ph.D. in engineering had not occurred to me. I am the first in my immediate family to pursue any level of degree in STEM, so I was already in uncharted territory. I had an interest in research, but no plan for a direction to pursue. This all changed in my sophomore year Physics of Materials class, which introduced me to computational chemistry and materials science. I was immediately fascinated by this topic, and I spent the remainder of my undergraduate studies seeking out research and coursework to learn more about it. I enjoy learning things that are already known to others, but I ultimately chose to pursue a Ph.D. to conduct research that expands the boundaries of human knowledge. Specifically, I came to MIT to develop new ways of coordinating computational and experimental tools for the high-throughput discovery of new chemistry and materials. **My experiences in research, teaching, leadership, and mentorship have motivated me to pursue a career as a university professor. This career will allow me to advance scientific understanding through open-access research and to inspire the next generation of scientists and engineers through inclusive teaching and mentorship.**

I sought out my first experience in computational research in the summer after I was introduced to the field in my Physics of Materials class. I was selected for the Summer Undergraduate Research Experience fellowship at U-M, which I used to work with a Ph.D. student in the group of Prof. Katsuyo Thornton. The goal of our work was to simulate cathode nanoparticles of various shapes and constituent materials to improve Li-ion batteries. I designed a parametric study to determine the independent effects of several material properties, and I learned how to use high-performance computing (HPC) resources and to visualize data from simulations. My work showed the potential of certain hybrid cathode materials to improve electrochemical performance when paired together in the right way. This could impact the design of new rechargeable batteries for transportation applications and make electric vehicles more economical. After a summer working on this project, I confirmed my interest in computational materials science research and began to consider the possibility of pursuing a Ph.D.

I enjoyed my work with continuum-scale simulations, but I was interested in expanding my computational toolkit to include first-principles calculations. At the beginning of my junior year, I started working in the group of Prof. Manos Kioupakis at U-M using density functional theory (DFT) to study the properties of semiconductor alloys. When I first began this work, I struggled with the repetitive nature of my calculations, which led me to teach myself more advanced Bash scripting to automate pre- and post-processing tasks. This automation enabled me to explore the effects of adding boron to indium-gallium-nitride (InGaN) by using DFT to study the entire composition space and find the most stable crystal structure at each composition. This research could one day improve the cost-effectiveness of commercially available light-emitting diodes (LEDs), which would increase their adoption and lower energy usage. **I published a paper on this work in the *Journal of Applied Physics* as first author, and I gave an oral presentation on it at the 2019 American Physical Society March Meeting.** This experience helped develop my knowledge of DFT and enhance my ability to utilize HPC resources effectively. Along the way, I grew in my independence as a researcher through taking ownership of a project and learning to communicate my work.

In the summer after my junior year, I was selected to work with Prof. Peilin Liao in the NSF-funded Network for Computational Nanotechnology at Purdue University. I used the knowledge of DFT I had been developing in Prof. Kioupakis's group to create a new tool on nanoHUB.org for calculating descriptor properties in heterogeneous catalysis. While catalysis has been studied using DFT for many years, there has never been a publicly-available, user-friendly tool for doing so that could be used within a web browser. Access to the proper software packages and HPC resources can present a barrier to individuals interested in this research field, but my tool alleviates this issue by allowing anyone to use it free-of-charge. I taught myself how to use several software packages and libraries to help build the tool and took the initiative to overhaul the user interface to make the tool more usable in both research and education. **As of this writing, my tool has had over 250 users across five continents since its publication two years ago. I worked on this project independently and published the tool as first author.** After this second summer doing full-time research, I became certain that a Ph.D. was the right path for me because I thoroughly enjoyed the freedom to teach myself new skills while leading a research project. Furthermore, I learned about the positive impact that open-source tools can have on research and education and resolved to make this an integral part of my future work.

I matriculated into MIT this past fall to begin my Ph.D. in the Chemical Engineering and Computation joint program. I joined the groups of Profs. Rafael Gómez-Bombarelli and William Green because my undergraduate research taught me about the limitations of computational work without experimental collaboration, and these two groups had strong relationships with experimental collaborators in addition to their expertise in physics-based calculations and machine learning. My work now focuses on developing methods to coordinate the interplay between experimental data, atomistic calculations, and machine learning for the discovery and design of new dye molecules for biomedical sensing and diagnostics. I am well-equipped to conduct this research through my two years of undergraduate research using DFT and my coursework in data science. Since joining these groups in January, I have led an effort that has achieved a world-best performance on predicting the wavelength of maximum absorption based on a dye's molecular structure. **I will soon be publishing a preprint on this work as first author and making my data and code openly accessible in the interest of reproducibility.** I will continue this work with the eventual goal of creating a platform that will extend beyond dye molecules and accelerate the discovery and design process throughout the fields of chemistry and materials science.

In addition to research, my teaching experiences have played a significant role in shaping my desire to become a professor. As a study group facilitator for organic chemistry, I led a group of thirteen students to review concepts and practice problems in weekly review sessions. I enjoyed this and decided to challenge myself in a bigger role as an instructional aide for fluid mechanics, which came with the responsibility of leading a weekly review lecture for over 100 students. My most significant teaching experience came in my senior year when I was a leader in an initiative to establish a new chemical engineering elective class at U-M. The class was designed to expose underclassmen to the variety of research occurring in the department and give them basic skills in each area. **I led a group of several undergraduate and graduate students in planning the second half of the new course, which focused on techniques in computational research.** My team wanted to inspire departments at other schools to enact similar initiatives in their curricula, so **we published a paper describing our class in *Chemical Engineering Education*. I contributed as second author to this paper.** From this work, I learned that incorporating current research into an undergraduate curriculum can positively benefit student engagement in the classroom, as well as motivate students to seek out research opportunities outside the classroom. These experiences have prepared me to serve as an instructor during graduate school and reaffirmed my desire to become a professor who will integrate research into the curriculum and engage undergraduates in research.

I have extensive leadership experience that supplements my research and teaching. My most significant involvement was in Tau Beta Pi (TBP), the engineering honor society. I was elected to serve terms as the chapter Professional Development Officer and President. As President, I developed my ability to lead a diverse team as I managed seventeen officers to carry out all of our chapter's programming and operations. This included engaging approximately two hundred undergraduate and graduate student members in service, social, and professional development activities. In addition, I focused on improving diversity, equity, and inclusion within the chapter (e.g., by creating a mentorship program and an initiation fee waiver application). Beyond TBP, **I worked with six other undergraduates in my senior year at U-M to create the first campus-wide Undergraduate Research Symposium (URS), which gave a venue for nearly 150 undergraduates to present posters.** We raised over $12,000 in funding for the event, much of which went toward travel awards for ten students to present their work at off-campus conferences of their choice. I look forward to using the knowledge and experience I have gained through leadership in TBP and the URS to promote diversity, equity, and inclusion and to expand access and opportunities for undergraduate research during my graduate studies and in my career as a professor.

At MIT, I have become involved in mentorship activities in my department and beyond. I am now in my second year serving as a mentor for students from underrepresented backgrounds applying to the Ph.D. program in chemical engineering. I use this role to provide feedback on students' applications and answer their questions about the department and graduate school in general. I have also engaged in mentorship outside of the Institute. For example, I joined the Netpals program through the Cambridge

Public Schools system to help seventh-grade students practice using professional communication skills and learn more about STEM careers. **I will continue to contribute my time to mentorship throughout my career because I recognize that it plays an integral role in recruiting and retaining diverse talent in academia and cultivates an interest in and appreciation of science in the broader community.**

Intellectual Merit My two years of experience with density functional theory and high-performance computing will be invaluable as I continue in research that relies heavily on both. My work has resulted in a first-author paper in the *Journal of Applied Physics*, an oral presentation at the American Physical Society March Meeting, a first-author open-source tool for research and education on nanoHUB, and several poster presentations. I will leverage this experience as I continue to improve my ability to communicate my work in graduate school, beginning with my ongoing preparation of a first-author preprint on my current research at MIT. I have engaged in teaching by facilitating small organic chemistry study groups, leading review lectures for a large fluid mechanics class, and designing and teaching a new class in my undergraduate department. I have begun developing my own philosophy on teaching and education, which I communicated in part as the second author on an article in *Chemical Engineering Education*. These experiences in teaching have given me a strong foundation that complements my technical skill set and prepares me to be a leader in my future academic career.

Broader Impact My previous research has advanced several fields of great interest to society, including Li-ion batteries for higher-capacity energy storage, catalysis for chemical and energy production, and LEDs for more efficient lighting. My current research will enable greater collaboration between experimental and computational researchers while accelerating the design of new molecules and materials. Throughout my career, I will choose research topics with transformative potential and **make all datasets, codes, and tools I create freely accessible to enable other researchers to easily reproduce and build on my work.** While I have chosen to work on impactful problems in science, I recognize that many people face barriers that hinder their access to participation in STEM. This has led me to create and participate in initiatives to address this problem. For example, I designed and taught a new undergraduate course seeking to increase awareness of and interest in research, created an initiation fee waiver process for my Tau Beta Pi chapter, and founded a campus-wide research symposium that gave 150 undergraduates an opportunity to present their work on campus and funded travel awards for ten students to present their work at professional conferences. I have also engaged in mentorship programs to increase middle school students' interest in STEM careers and to assist underrepresented students with the graduate school application process. I will build on this work during graduate school by **mentoring undergraduate researchers** and continuing to contribute to programs that expand access to STEM.

Future Goals My time at MIT will enable me to enhance my teaching and leadership skills. I plan to serve as a teaching assistant during the course of my Ph.D. and will complement this experience with pedagogical training. I began this training this past summer by completing the Subject Design Certificate Program through MIT's Teaching and Learning Lab, where I learned important lessons on effective and inclusive course design. I also plan to join MIT's Kaufman Teaching Certificate Program (KTCP), where I will have the opportunity to practice my teaching skills in workshops and receive feedback from peers and experts. I will also pursue a Graduate Certificate in Technical Leadership at MIT to better prepare me to be an effective leader of an academic research group.

Previous research and teaching activities have informed my goal of becoming a professor, and I have begun my Ph.D. as the next step toward achieving this goal. My Ph.D. research is preparing me to be a future leader in techniques for integrating experimental and computational approaches to chemical discovery. Few things excite me as much as the potential to discover new things, but one thing that comes close is the opportunity to positively influence the lives of others through teaching and mentorship. A career as a professor would allow me to do impactful research while also inspiring and empowering the next generation of scientists and engineers. **Receiving an NSF Graduate Research Fellowship would allow me to pursue my research and professional goals unencumbered by uncertainties or shortfalls in funding. It would give me the flexibility to engage in the teaching, leadership, and mentorship activities that will complement my research work as I develop myself holistically to prepare for my future career as a professor.**