My interest in research and education arises from my grandmother, a nursing assistant with a passionate interest in chemistry and physics. Her infectious enthusiasm for education defined my childhood, whether it would be explaining electrostatic precipitators as we passed smokestacks of a coal plant, or calling me from work to talk about the discovery of the Higgs Boson. While my grandma was never able to pursue education, I know she would have been an amazing scientist, and I work harder knowing I'm pursuing both of our dreams. As a first-gen/low-income college student from rural western Wisconsin, my success is completely indebted to having caring and strong mentors that helped me realize my path. This journey started in my honors general chemistry laboratory, where my undergraduate research mentor, Dr. Bhattacharyay, offered me a position in his computational chemistry group. Although the learning curve was incredibly steep for a first-year student, my curiosity and self-instruction allowed me to keep up, and I presented my first research poster at the end of the semester.

This initial project focused on investigating π-π stacking interactions in flavin-aromatic complexes, which are very prevalent in biological systems. I performed a series of quantum chemical calculations, benchmarking the dependence of the quantitative agreement with experiment on the density functional and basis set. This work came to fruition in the form of a publication, which was the first step in building my confidence in my career. The paper entitled "Effects of Stacking Interactions on the Thermodynamics and Kinetics of Lumiflavin: A Study with Improved Density Functionals and Density Functional Tight-Binding Protocol" was published in the *Journal of Physical Chemistry A* in early 2015, with myself as co-first author. Experiencing the review process and amount of work that goes into a publication early in my undergraduate career ignited my passion for research.

Following this work, I approached Dr. Bhattacharyay suggesting that we complete a project started by the students of one of his physical chemistry courses. This work focused on hydride transfer reactions between flavin and substituted quinones, scrutinizing the effect of substituents on shifting the transition state towards a more reactant or product-like configuration. My second first-author publication, entitled "Insight into the Kinetics and Thermodynamics of the Hydride Transfer Reactions between Quinones and Lumiflavin: A Density Functional Theory," was published in the *Journal of Molecular Modeling* in August 2016. This work exposed me to difficult concepts of physical chemistry and pushed me toward becoming a more independent researcher as I had to respond and address reviewer concerns while my advisor was abroad for a family emergency.

While I enjoyed working with small models, I was excited to use my biology background and model an enzyme complex with hybrid quantum mechanical/molecular mechanical (QM/MM) simulations. Quinone reductase II uses a single set of active site residues to catalyze opposing hydride transfers, so our study focused on addressing the response of the local environment to redox changes. Using enhanced sampling techniques, I determined the Gibbs free energies of reaction. Then I assisted with analyzing the essential dynamics of the protein, producing both a local picture of the active site and a global picture of the overall role of protein motion. I was delighted when I had enough data to present at the national American Chemical Society (ACS) meeting in spring 2016 and submitted an abstract.

Participation in the 249th ACS meeting in Denver was perhaps the most critical step in my development to date. While I had submitted an abstract for a poster, I instead found myself with an opportunity to give an oral presentation. I was a sophomore at the time, so I worked to prepare and practice between classes and the off-campus job I held. I presented the talk entitled "Quantum Mechanical/Molecular Mechanical Simulations of the Hydride Transfer Reactions in Quinone Reductase 2" within the computational chemical dynamics symposium in honor of Donald Truhlar. My talk was well received, and my advisor pushed me to write up the manuscript, which is currently under the 2nd round of review for *ACS Catalysis* as of October 2018.

The summer after the Denver meeting greatly strengthened my ability to think critically and creatively to solve research problems working under minimal supervision. I encountered a challenge arising from trying to develop a standardized docking protocol for inhibitors. My mentor and I bounced ideas off each other daily, but like most research plateaus, those days became weeks. Finally, we produced a geometric docking algorithm that would allow us to introduce molecules without a commercial package. Three months later, I presented this work at the 251st ACS National Meeting in San Diego and was awarded the "Excellence in an Undergraduate Research Presentation" in the Computers in Chemistry Division. Following this award, I was selected as the region's "Outstanding College Chemistry Student" by the Central Wisconsin Section of the ACS.

While these accolades validated my hard work, I have not forgotten where I started my journey. As a first-generation college student from an economically disadvantaged family, I cannot picture where I would be without the support and opportunities I have received from the faculty, the campus community, and the Ronald E. McNair Postbaccalaureate Achievement Program. I decided to return to my former high school and give presentations to high school science classes about research and academic opportunities in college. While my presentations were geared toward motivating STEM majors, I worked to present material relevant to all students considering college. I went on to start an outreach program through the American Chemical Society to inspire other college STEM students to give similar presentations to local high schools. While the program is small, due to the sheer amount of work required in starting a new initiative, I believe it is addressing the socioeconomic barrier in attending college present in the area.

My transformation in college and my experiences mentoring younger students in the research lab led me to apply for a position leading a required freshman Honors student seminar course. Collaborating with a fellow Honors student, I constructed a syllabus, arranged for speakers, designed assignments, and had weekly feedback and discussion meetings with the Honors program director to monitor progress. This experience confirmed my joy in the educational process and solidified my interest in becoming a professor. After this exposure to a classroom setting, I began to blend my interest in education with my interest in research and designed and taught a project for the biophysical chemistry course. I wrote instructions and taught the background material in the lab section, and then I helped students set up a hybrid QM/MM molecular dynamics simulation using methods in our lab. I integrated the geometric docking protocol to allow them to introduce their own inhibitors, giving them ownership and a unique project that I hoped would boost interest. I started compiling these results and methodologies into a manuscript before my departure to graduate school.

I tied up my final year by writing a University Honors Program thesis, which made me only the second UW–Eau Claire student to do so, and the first for the Chemistry Department. I wrote a six-chapter thesis, four chapters consisting of my intellectual contributions to each distinct project and two chapters summarizing the theoretical background of our methodology and biological systems, which ended up being more than 100 pages. I would be giving an inaccurate picture of science if I claimed this process was all rosy, as I did not maintain consistent mathematical notation, and my committee member drenched those pages in red ink. This experience taught me that revision and careful reading by a conscientious eye are traits to be continually honed. I took this lesson and prepared the final draft and defense presentation diligently, reminding myself that there is always room for growth.

Upon arriving to Yale, I immediately became involved with outreach and teaching. I began in the summer upon my arrival by interjecting myself into the physical engineering biology programs' outreach efforts, developing my own exercise and presentation to middle school students on the physical properties of proteins. In tandem, I joined the graduate outreach organization called Open Labs and became the finance chair. Upon joining the organization, I was informed that a large grant for $10,000 was awarded two years prior, but the point of contact was non-responsive. Viewing this as unacceptable and a block to exposing kids to science, I sent a series of more than 30 emails and obtained a signed contract from the awarding agency to contract us the funds. We hold multiple events per year reaching over 200 kids, but with these funds we can expand our scientific demo infrastructure and host more school kids at each event.

The identification and elimination of roadblocks to learning is not only limited to working with younger peers. As I proceeded through my graduate coursework, I also identified that a discussion-based literature class was lopsided by inconsistencies in discussion etiquette among the incoming participants. My colleague and I drafted a proposal for a four-session workshop to be implemented before the course to properly train students on effective scientific discussion, allowing all users to benefit from this literature course. This training course has been approved, and we will teach it this spring. I have continued to develop my teaching abilities by serving as a lead instructor for Yale Young Global Scholars, which brings bright high school students to New Haven for an intense two weeks of academic development. In this experience I developed six 90-minute seminars on topics of my choice, which ranged from computer-aided drug design, to quantum mechanics in biology, to diversity in science.

Although I am very active with outreach and teaching in graduate school, I do not let these activities interfere with my research progress. I joined Dr. Sharon Hammes-Schiffer's lab in the Spring of 2018, initially studying an active-site tryptophan residue in the blue light-using flavin photoreceptor protein. This residue was proposed to play a key role in the photocycle, but its conformation within the active site is debated because of conflicting structural data. Through enhanced sampling methods, I was able to show that the free energy barrier for interconversion between the two observed tryptophan conformations was prohibitively high, suggesting that the conformations do not interchange during the photocycle and instead can be attributed to either crystallization or differential protein folding. This work was incorporated into a manuscript recently published in the *Journal of the American Chemical Society*, for which I am the second author. In my thesis work, I am studying proton-coupled electron transfer (PCET) reactions involving tyrosine and tryptophan residues, which are important to processes such as photosynthesis, cellular respiration, and the synthesis of DNA. However, the role of the protein environment in controlling these PCET reactions is not well studied. An NSF fellowship would enable me to continue to explore these fundamental aspects of biological PCET reactions, and to continue my work engaging the next generation of scientists.