As a young person, I want to be part of the effort to adapt to climate change. As a scientist, I am interested in the numerical methods of quantum chemistry. These two desires can be reconciled at *this school* by developing computational methods for elucidating the electronic structure of correlated materials used in sustainable fuel and chemical production. Working towards a PhD here will enable me to attain my future goal of teaching as a professor at a research institution.

My journey started with the freshman general chemistry class. Learning about how the local geometry of electron orbits affects global chemical properties was fascinating.

Immediately after my freshman year, in 2019, I performed research througha Summer Undergraduate Research Fellowship (SURF) in Prof. Ryan G. Hadt’s physical inorganic chemistry laboratory at Caltech. During my research, I developed a computational protocol for characterizing mechanisms of spin-phonon coupling in Co(III) complexes relevant for quantum information science. I first used DFT with atomic orbital basis sets to optimize geometric structures and to obtain the vibrational normal modes. Next I determined which modes were relevant to spin-phonon coupling. Because the excited states of these open-shell first-row transition metal-containing systems have significant dynamic electron correlation, our research required the use of multireference methods for quantitative accuracy; hence, I used CASSCF with a perturbative NEVPT2 correction to investigate the energetics of spin crossover events along modes of interest. I found myself extremely interested in what was going on under the hood of the quantum chemistry methods that I was using. Whenever my calculations were running, I would enthusiastically ask my graduate student mentor to recommend reading in this direction. I enjoyed reading the relevant quantum mechanics sections Donald McQuarrie’s physical chemistry textbook; but what I especially enjoyed was reading sections of Szabo and Ostlunds’ graduate-level textbook *Modern Quantum Chemistry*. After discovering my passion for chemical theory and especially electronic structure,the coursework I took afterwards was geared towards theoretical chemistry, which included taking the physical chemistry sequence and a statistical mechanics class. I continued working on the project during the academic year and my work was subsequently included in a Journal of Chemical Physics publication.

After my sophomore year, in 2020, I did a SURF in Prog. Garnet Chan’s quantum chemistry group at Caltech. I computed surface energies of a platinum (111) surface, which is used as a heterogeneous catalyst in the Haber-Bosch process for the sustainable production of fertilizers. First, I used plane-wave DFT to corroborate literature about the method's overestimation of surface stability. Then, I ran MP2 and CCSD calculations on this system. With my limited timeline and computational resources, I was not able to overcome the inadequacy of DFT with MP2 and CCSD. Thus, I learned about the motivation for the research direction in quantum chemistry, which is to achieve accuracy in complex systems, such as periodic ones, without calculations becoming too expensive. I want to improve the performance of wave function based methods for periodic systems in my graduate training. I continued my reading of Szabo and Ostlund, focusing on the standard models of the field, perturbative approaches, and Green’s function methods. The coursework that I took afterwards was designed to teach me the toolkit to succeed in quantum chemistry, which included applied linear algebra and quantum physics courses.

In the fall quarter of my junior year in 2020, I worked remotely as a TA for an introductory quantum mechanics course for chemists. It was the first year that Prof. Mitchio Okumura was teaching the course and he was refreshingly concerned about students’ understanding of the material. Along with the other TAs, I met with him weekly to discuss what aspects of the lecture students were struggling with, and how we could design our recitations to address this. I thoroughly enjoyed the challenge of explaining complex concepts to students, which is something I would like to continue in graduate school and beyond.

Throughout this quarter, I also wrote a publication for the Caltech Undergraduate Research Journal describing the findings from my SURF of the previous summer. This and my TA experience sharpened my scientific communication skills for conveying high-level concepts to non-technical audiences.

At the beginning of the winter quarter of my junior year in 2021, I was diagnosed with leukemia and, subsequently, suffered a stroke. My cognitive faculties were left untouched, but I have motor deficits. I was initially bed-bound and could not communicate. After 2 years of intense rehabilitation on medical leave, the improved presentation is that I use an assistive device, like a walker, to ambulate. Typing and handwriting are impractical due to my impaired fine motor function, and I have spastic dysarthria, meaning that I have weakness in my articulators, a slower rate of speech, and difficulty changing pitch. The fortitude that has been required of me to succeed in rehabilitation has taught me the perseverance that will aid me in graduate school.

My return to academics has been made possible by artificial intelligence, which allows me to do science as if nothing ever happened. In addition to powering the dictation software that I use, it is behind GitHub Co-Pilot, which makes suggestions for me as I write code. And I use ChatGPT for a variety of purposes, ranging from correcting typos in my dictated prose to helping me understand my code better. My ability to voice code using AI has only reinforced my desire to pursue theoretical chemistry and makes me confident that I can succeed in this field in graduate school.

This past summer, I implemented and optimized Full Configuration Interaction (FCI) for a simple H6 chain under the supervision of Prof. Garnet Chan. This project has introduced me to dealing with the standard problem of quantum chemistry, namely of large, sparse matrices. I have implemented the Davidson algorithm in order to just compute the few desired eigenvalues of the FCI matrix and also the algorithm of Handy & Knowles (1984), which uses the one-particle matrix to circumvent generating the FCI matrix altogether.

I will be continuing with Prof. Garnet Chan for a senior thesis, where I will be doing *these things.*

**Insert tailoring paragraph here.**