STATEMENT OF GRANT PURPOSE
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Electronic structure at King's College London

First, I should address the fact that I am applying for a graduate degree in physics, even though my undergraduate degree is in chemistry. My research interest is in theoretical chemistry, which is at the intersection of physics and chemistry. The program specific requirements for the physics MSc at King's state that: "Alternatively...a degree subject related to physics will be considered on a case by case basis." The coursework I have completed in my chemistry undergraduate degree should be more than sufficient, given Caltech's theoretical leaning in the field.

Because of the medical leave from my stroke, I am returning to Caltech for my senior year to finish my B.S. degree without having much flexibility to take the physics courses of interest that I would take had I not been out on leave. The KCL graduate degree in physics will allow me to fill in these gaps. Additionally, the way in which higher education differs in the UK versus the US works to my advantage. In the UK, obtaining an undergraduate degree takes three years after which a student typically does a one-year master's program, like the one here, before pursuing a PhD. This graduate program would serve as an ideal bridge between my undergraduate studies and a physics-minded PhD program in electronic structure. I want to study at King's College, which is at the heart of London, not only for accessibility reasons, but also because my proposed research supervisor, Prof. Booth, is an expert in electronic structure, which I want to continue studying in my later graduate studies in America. I have completed coursework in quantum and statistical physics and will continue to do so during my senior year, which will prepare me for this graduate program. Prof. Booth and I have worked out a doable research project for my MSc, which I have detailed below. I have been upfront with him about my speech and mobility issues and he is very supportive.

The breakdown for the program is as follows: the requirement is for my total units taken for the year to amount to 180. To give an idea, "Typically, one credit equates to 10 hours of work, e.g., 150 hours work for a 15-credit module." I will satisfy this requirement with the following. I will conduct a research project with Prof. Booth and my completion of this project will culminate with a dissertation. Another required module is scientific communication, where I will learn to work with a variety of audiences through different media, such as radio, video, newspaper articles, and social media. This module is forward thinking in our age of social media. Additionally, I will take modules at King's College in the Theoretical Treatment of Nano Systems, Advanced Condensed Matter, Modeling Quantum Many-Body Systems, and Simulation Methods for Nonequilibrium Systems. I will also be choosing from a wide selection of modules offered at partner universities in the University of London, such as Superconductivity, Superfluids, and Condensates, as well as Quantum Computation.

Computation is an essential tool for the modern chemist. In particular, there is a focus on *ab initio* methods, which has the Latin meaning of "from the beginning." What this means is that these calculations are not empirically based and are starting from scratch; an understanding of the inherent physics involved in the system is being used to compute global chemical properties. I have experience in applying these methods. In the research internship after my freshman year, I studied transition metal complexes computationally to gain insight for experimental spectroscopists. The primary focus of this field, known as theoretical chemistry, is to maintain the accuracy of such computational methods, while reducing the time they take to run. For example, from my research experience, when the focus is on achieving accuracy on par with that of the experimental literature, calculations can take days to weeks to run. This summer of 2023, I am learning theoretical chemistry by implementing a computational method called Full Configuration Interaction (FCI). However, in my case, I am designing my program to be able to deal with a chain of 6 hydrogen atoms, comprised of only 6 electrons, and running it all on my personal computer.

As one can imagine, chemists, with supercomputers at their disposal, are interested in studying more complex systems. However, even so, computational resources only scale linearly, while FCI scales exponentially with the system size. FCI is known to be accurate, but it is primarily used for benchmarking other theoretical chemistry methods, as using it to compute properties of larger systems of interest, such as proteins, can take months to years to run. Prof. Booth is developing a new method called FCI Quantum Monte Carlo. The Monte Carlo part of the name indicates that it is a stochastic, or probabilistic, method and can, therefore, deal with much larger systems. Furthermore, FCI QMC has shown an ability to still accurately capture critical properties. This method has shown potential in dealing with correlated materials. Correlated materials exhibit a wide variety of unusual, and technologically useful, properties. Many of them are being used for sustainable chemical and fuel production. For them, simply averaging the effect of the "sea" of the other electrons on an electron is not enough (this is called a mean-field approach where only the cumulative effect of the other electrons in the system is being considered). Rather, the complex interactions between the electron and each of its neighbors matters. I can utilize my skills learned in the FCI project to create a computationally more efficient implementation of FCI QMC in my research project at King's. Additionally, the coursework offered in this physics MSc will prepare me to be successful with a research career in electronic structure.