**Statement of Purpose**

Can Li

Born and raised up in Jiaozuo, China, a small industrialized city badly affected by pollution, I have witnessed the worst scenario of inefficiencies in chemical processes. I am determined to make a contribution in science to help alleviate many of these similar problems that affect us collectively as a global society. I am strongly motivated to pursue a scientific career and getting PhD is the first step towards it. Specially, I am interested in working on process systems engineering.

I decided to major in Chemical Engineering at Tsinghua University in 2012 as an undergraduate. In addition to attending strong courses within Chemical Engineering Department in which professors covered both the breadth and depth of chemical engineering fundamentals, I took various classes on computer programming. The power of computing and elegance of algorithms completely intrigued me. Having interest in both chemical engineering as well as computer programming motivated me to work at the intersection of computations and chemical engineering.

The strong passion for scientific research incentivized me to join the lab of Prof. Yushan Zhu when I was a sophomore, where I worked on computational design for a new enzyme that could catalyze the acylation reaction in cefataxime synthesis. As there is no mature design protocol in this area, I managed to set up my own standard to evaluate each design and the distance of the nucleophilic attack, the distances of two hydrogen bonds stabilizing the transition state and a docking score were employed to evaluate the docking outputs. I applied both one-residue sampling and a trial-and-error approaches to find mutations that could make the enzyme-ligand complex satisfy all our geometric constraints. Finally, a new enzyme satisfying all the geometric constraints and showing high docking score with five-residue mutations was found to bind cefataxime well *in silica*. This experience definitely gave me a big picture of how to make hypothesis and how to find the reasonable method to solve the problem based on the hypothesis in scientific research.

Owing to my strong academic performance, I was awarded to study at UW-Madison for fall semester of 2014, where I not only got firsthand experience of the course study and research in American graduate school, but also deepened my understanding of computation in chemical engineering. I took *Advanced Chemical Engineering Thermodynamics* class wherein I not only learned statistical mechanics and molecular simulation, but also discussed representative papers about Monte Carlo and Molecular Dynamics simulation with Prof. Nicholas Abbott and other PhD students. I also joined Prof. Christos Maravelias’ Process Systems Engineering group where I learned mathematical models and algorithms of Linear Programming and Mixed Integer Linear Programming problems. I tried to emulate the current best model for scheduling of multistage batch process under utility constraints with discrete-time formulation (Sundaramoorthy (2009)) by using continuous-time formation and built three new models. The correctness of my models was validated by solving sample problems, but I could not validate the efficiency of the models primarily due to my limited ability to do root cause analysis using advanced mixed integer programming theory. However, this motivated me to take more courses in numerical optimization and computer programming back at Tsinghua University. I have done various course projects which enhanced my capability to solve practical computational problems. I’m taking *Numerical Analysis, Algorithm Design, Machine Learning,* and *Software Engineering* in the fall semester of 2015.

In order to be exposed to the frontiers of research, I had an internship in Prof. David Baker’s Lab at University of Washington this summer. I worked with a graduate student on de novo design of protein fiber using Rosetta, the computational tool of Baker Lab. We first docked our building blocks, someαhelical bundles, into helical structure, after which over five thousand docking structures were obtained and were ranked by their second largest interacting surface area. I selectively visualized 20% of the output structures and classified the docking structures into four topologies. I selected 26 structures with “good” topologies and interacting surface areas based on previous experience of the lab. My heuristics proved to be helpful after the graduate student run the further design protocol, which would output hundreds of thousands of design structures, laborious and intimidating for manual selection. Actually, he found excellent designs using the docking structures I selected. Moreover, after he used the 26 structures as training data to calibrate the parameters of the filter, more “good” docking structures were found and were in the process of design. My research experience in United States has also well prepared me to communicate and collaborate with people from different cultures and academic background.

I was extremely amazed at the power of computation when I visualized one fiber-shaped order using transmission electron microscopy, when I significantly increased the profit using the scheduling models and when I imagined one computationally designed enzyme might replace a traditional chemical process. I love the life of consistently learning, discovering and evolving. That is why I decided to pursue a PhD degree. UW-Madison CBE PhD program has a solid curricula and faculty working on my interested research areas. I’m especially interested in Dr. Christos Maravelias and Dr. Victor Zavala’s work on computational optimization. I admire Dr. James Rawlings, one of the recognized leaders in control theory. My background also pertains to the work of Dr. Jennifer Reed and Dr. Michael Graham.

After receiving a PhD degree, I plan to be a leading scientist in academia contributing to the advancement of energy conservation and environment protection. I look forward to collaborating with colleague on solving complex problems, and guiding students through the excited process of scientific discovery. Furthermore, I will facilitate cross-cultural understanding and transnational collaboration as a global citizen.