**Statement of Purpose**

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Mesmerized by the magic power of chemistry, I chose to become a member of the Chemistry Olympiad Class when I was in high school and ended up with the first place of Henan province in National Chemistry Olympiad. At the awarding lecture, Prof. Xi Zhang (Chair of Department of Chemistry, Tsinghua University) said something that I never forget: ‘though human being has made great progress in chemistry, we are still far from being able to design molecules as we wish. This piqued my curiosity to find the underlying molecular driving forces and made me pursue a scientific career.

I decided to major in Chemical Engineering at Tsinghua University in 2012 as an undergraduate. The strong passion for scientific research motivated 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. I used the distance of the nucleophilic attack, the distances of two hydrogen bonds stabilizing the transition state and a docking score 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 got firsthand experience of both the course study and research in American graduate school. To understand the fundamental theories and techniques in molecular design, I took *Advanced Chemical Engineering Thermodynamics* 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 emulated the current best model for scheduling of multistage batch process under utility constraints with discrete time formulation by using continuous time formation. I built three new models and the correctness of my new models was validated by solving sample problems. This experience enhanced my capability for modeling and enriched my knowledge for numerical optimization, which are indispensable as a computational scientist in molecular engineering. The efforts I have paid to strengthen my computation and mathematical background are not limited to that. I have done various course projects which made me more capable of solving practical computational problems. I’m taking *Numerical Analysis, Algorithm Design, Machine Learning,* and *Software Engineering* in the fall semester of 2015. All I want is that I will be qualified as a PhD candidate in developing new methods useful in designing molecules.

In order to be exposed to the frontiers of protein design, 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 ranked by their second largest interacting surface area. I selectively visualized 20% of the output structures and classified the docking structures into four topologies. Among them, 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. He also 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. I also worked with the graduate student to express and purify recombinant proteins in *E.coli*. The purified proteins were characterized using TEM and one protein sample displayed fiber-shaped structure. I’m more passionate about protein design when I saw the amazing progress we made on building fibers. Besides, my research experience in United States has also well prepared me to communicate and collaborate with people from different cultures and academic background.

UW MolE program has not only solid curricula on molecular design, synthesis, and characterization but also faculty working on my interested areas. I’m especially interested in Dr. David Baker’s work on computational protein design and experimental characterization. I admire Dr. Valerie Daggett, one of the leaders in using computational method to design diagnostic and therapeutic agents to target amyloid diseases. My background also pertains to Dr. Jim Pfaendtner’s work on computational enzymology and molecular simulation.

After receiving a PhD degree, I plan to be a leading scientist in academia. I am enthusiastic about making my own contributions to unmask the underlying mechanism of molecular interaction and improve the design methods. I look forward to collaborating with colleague on solving design 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.