

Research Overview

The research component of this program is designed to meet the need of technical students who have a laboratory, research or capstone requirement. For practical reasons we will emphasize computational projects, but this is not a requirement. There are opportunities for laboratory experiences that can be discussed individually with the Director.

Computational projects involve the use of molecular dynamics or quantum chemistry to solve problems of interest to research groups at Zhejiang University. Since these groups collaborate with the Director there are components that will be initiated at NCSU. This is an integrated program that will involve preparation at NCSU followed by intensive work with Zhejiang University graduate students and professors. The level of expertise that the students will experience is extremely high. This is a unique opportunity to work closely with expert researchers. Chinese graduate students are anxious to meet U.S. students. Nowadays, the level of English language spoken is very high. There will not be a problem with communication. The Director will emphasize to the Chinese students the value of instructing the U.S. students in Chinese as a component of the program. This is a great way for them to improve their English while helping U.S. students acclimate. While there is no language requirement for this program, there will be ample opportunity for interested students to learn rudimentary Chinese in a unique method. The Director speaks Chinese and will also provide basic instruction in "Survival Chinese".

Students can learn either molecular dynamics (MD) or the quantum chemical method, density functional theory (DFT). The code used is freeware so that students will be able to use the skills gained in any computational environment, once they have learned the basics.

The MD code used is VMD/NAMD written and distributed by the Schulten group at the University of Illinois. VMD is a GUI interface that is easy to use and provides a powerful way to visualize proteins, DNA etc. NAMD stands for "Not Another Molecular Dynamics" code. Prof. Schulten has a sense of humor. His code is the fastest code written and runs very well on parallel environments. However, it can also run on a PC (just a little slowly).

The DFT code used is ORCA written and distributed by the Neese group at the University of Bonn. ORCA has become a versatile code that can be used for structure and spectroscopy. It currently has over 3000 users worldwide. ORCA is widely used for the study of metal centers in catalysis, which will be our main application.

Research topics include (but are not limited to)

MD studies of receptor-binding in cell targeting studies.

MD studies of dynamics and mutational analysis of dehaloperoxidase and related enzymes.

DFT studies of oxidative metal enzymes and industrial oxidation catalysts.