

## I. CHEM 5490

Using high performance computers and available software packages, students will examine the use of quantum chemistry to explore chemical systems and reactions. Topics will include potential energy surface exploration, stationary point characterization and property assessment. The intent of this course is to provide students with both background knowledge and hands on usage of computational methods used in the chemical sciences. The course is broken into a sequence of modules that cover specific details associated with different types of calculations. To provide practice in running experiments, a model system will be used for lab exercises. Experiments using an extended model system will then form the basis for the term project.