Introduction:

The course teaches the art of quantum mechanical calculations from both the chemistry and physics point of view. It, thus, falls somewhere between a laboratory course and a lecture course. In a laboratory course, you must learn by doing, and it is more important that you learn how to run the equipment well and how to interpret the data than that you learn how a piece of equipment is constructed and what exactly is under its cover. Similarly, in this course, you will learn how to run various quantum codes correctly and how to interpret the output of the codes, but you will not necessarily need to know how each algorithm in the 100's of 1000's of lines of code works. On the other hand, you will learn the theories behind the computer codes, so that you will be able to interpret the output of the codes. You will also learn about applications of computational quantum mechanical methods, in order to understand their potential and scope. Finally, you will gain insight into the current research and development of these methods to know where the field is going and what to expect in the future.

Course Objectives:

- Learn a different approach to solving scientific and engineering problems: performing quantum mechanical calculations and understanding their scope, possibilities and limitations.
- Be able to perform calculations during your research at MIT, in Practice School, and in your future work. (Several students of this class have published papers in major journals based on their projects.)
- Gain a (partial) familiarity with the literature and be able to read it critically.
- Understand current research directions and possibilities.
Textbook:

There is no suitable textbook for this course. The best one still seems to be *Modern Quantum Chemistry* by Szabo and Ostlund, which is available at the Coop and "required" for the course. *Introduction to Quantum Chemistry* by Frank Jensen has similar material, but also includes a discussion of density functional theory and has a useful chapter, 12 "Transition State Theory and Statistical Mechanics." It also has helpful descriptions of many of the methods that Gaussian uses. It is available at the Coop and "recommended" for the course. Finally, see the References document for other helpful books, which are all on reserve.

Software:

Gaussian03: used to perform quantum mechanical calculations
GaussView: GUI, used to create job files, run jobs, and visualize output
CPMD: (more info on this to come by the end of the summer)

Hardware:

Project Athena: Sun and Linux

NCSA (National Computational Science Alliance):
   SGI Origin 2000 (796 processors)

Your laboratory or other MIT owned Sun and Linux machines

Grading:

Homework 30%
Participation 20%
Final Project 50%