

Chem 562

Fundamentals of Atomic and Molecular Quantum Mechanics

Instructor:

Xueyu Song

Lecture: 12:05-1:25pm at Gilman 1813; Office Hours:by appointment

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Syllabus:

- Brief review of some mathematical materials (Ch1 of Szabo).
- Many electron wave functions and operators(Ch2 of Szabo)
- The Hartree-Fock Approximation(Ch3 of Szabo)
- Brief Discussion of CI, MCSCF and GVB(Ch4 of Szabo)
- Many-body perturbation theory(Ch6 of Szabo)
- The one-particle many-body Green's function(Ch7 of Szabo)
- Quantum density functional theory(Ch3 and 7 of Parr and Yang)

This course teaches through examples. Homework is an integrated part of the course. Problems are assigned for roughly every three classes. You are encouraged to collaborate for your homework provided that you tried by yourself. There are one midterm and one final. The grade will be based on homework(30%), midterm(30%) and final(40%). The required textbook is *Modern quantum Chemistry* by A Szaba and N Ostlund. The density functional theory part is based on *Density-functional theory of atoms and molecules* by RG Parr and W Yang.

Canvas, <https://canvas.iastate.edu/>. This site provides access to the syllabus, general resources, announcements, answer keys, and other miscellaneous class materials.