

# Chem 561

## 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.

**Public Health:** If you are not feeling well, you should stay home and focus on your health. Should you miss class due to illness, it is your responsibility to work with your instructor to arrange for accommodations and to make up coursework, as consistent with the instructors attendance policy.

You may choose to wear a face mask and/or receive the COVID-19 vaccine and boosters, as well as other vaccines such as influenza, but those options are not required. Thiel Student Health Center will continue to provide COVID-19 vaccinations free-of-charge to students. The university will continue to offer free masks and COVID-19 test kits

during the fall 2022 semester. Other wellbeing resources for students are available at: <https://www.cyclonehealth.iastate.edu/wellbeing-resources/>.

Public health information for the campus community continues to be available on Iowa States public health website.

All public health questions should be directed to [publichealthteam@iastate.edu](mailto:publichealthteam@iastate.edu).

**Accessibility Statement:** Iowa State University is committed to assuring that all educational activities are free from discrimination and harassment based on disability status. Students requesting accommodations for a documented disability are required to work directly with staff in Student Accessibility Services (SAS) to establish eligibility and learn about related processes before accommodations will be identified. After eligibility is established, SAS staff will create and issue a Notification Letter for each course listing approved reasonable accommodations. This document will be made available to the student and instructor either electronically or in hard-copy every semester. Students and instructors are encouraged to review contents of the Notification Letters as early in the semester as possible to identify a specific, timely plan to deliver/receive the indicated accommodations. Reasonable accommodations are not retroactive in nature and are not intended to be an unfair advantage. Additional information or assistance is available online at [www.sas.dso.iastate.edu](http://www.sas.dso.iastate.edu), by contacting SAS staff by email at [accessibility@iastate.edu](mailto:accessibility@iastate.edu), or by calling 515-294-7220. Student Accessibility Services is a unit in the Dean of Students Office located at 1076 Student Services Building.