

Chemistry 421/521: Atomic and Molecular Structure

David Case, instructor. Office: 208B Proteomics, cell: 609-751-8668
email: david.case@rutgers.edu
Spring 2023, Mondays and Wednesdays, 2:00 to 3:20 pm, ARC-206

This is a one-semester physical chemistry course, covering quantum theory of molecular electronic structure. You should have completed undergraduate physical chemistry, such as CCB 327/328 here at Rutgers, or the equivalent elsewhere. This course will cover the basics of quantum mechanics and its applications to problems in electronic structure in chemistry.

The course text is Frank Pilar, *“Elementary Quantum Chemistry, 2nd edition”*, (Dover). (The “digital version” is very bad: please use the printed version.) There will be additional hand-outs for some topics. The table below gives an approximate time schedule; detailed reading assignments will be made as the class proceeds.

Week starting	Subject	Chapter
Jan 18, 23	Quantum mechanics of simple systems	1-4
Jan 30, Feb 6	The hydrogen atom	5
Feb 13, 20	Approximation methods	6
Feb 27	Electron spin and many-electron systems	7,8
Mar 6,20	The Hartree-Fock method	9,10
Mar 27, Apr 3	Molecular electronic structure	11-13
Apr, 10	Density functional theory	
Apr 17	Connections to spectroscopy	
Apr 24, May 1	Student project presentations	

The course website is <http://casegroup.rutgers.edu/lnotes.html>. Reading and homework assignments and additional course materials will be posted there. Final grades in the class will be based on assigned homework/problem sets (30%), exams (40%), and student presentations (30%). Midway through the semester, each student will chose a project, which can be related to research you are carrying out, or to some facet of quantum chemistry (broadly interpreted) that interests you. Students will be expected to make a short oral presentations to the rest of the class, as well as to attend and provide feedback to other student presentations. A written summary of the project will also be required. Two take-home exams will be given during the course of the semester and announced as least one week beforehand; there will not be an exam during the Final Exam period.

Please note: Students are expected to adhere the university policies on academic integrity and student conduct in all assignments, assessments and other matters regarding this course. You may consult with fellow students on homework and on class projects, but you must personally prepare and understand any written material you hand in. You may *not* consult with fellow students on the exams or the course project.

Rutgers University takes academic dishonesty very seriously. Academic dishonesty includes (but is not limited to):

- cheating

- plagiarism
- aiding others in committing a violation
- allowing others to use your work
- failure to cite sources correctly
- fabrication
- using another person's ideas or words without attribution
- re-using a previous assignment
- unauthorized collaboration
- sabotaging another student's work

If in doubt or unfamiliar with anything on this list, please consult the instructor. More information is available at <https://nbacademicintegrity.rutgers.edu/>.