

Chemistry 421/521: Atomic and Molecular Structure

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Spring 2022, Mondays and Thursdays, 10:20 to 11:40am, CCB 1209

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). There will be additional handouts 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 20, 24	Quantum mechanics of simple systems	1-4
Feb 7	The hydrogen atom	5
Feb 14, 21	Approximation methods	6
Feb 28	Electron spin and many-electron systems	7,8
Mar 7,21	The Hartree-Fock method	9,10
Mar 28, Apr 4	Molecular electronic structure	11-13
Apr, 11	Density functional theory	
Apr 18	Connections to spectroscopy	
Apr 25, May 2	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%).

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, but you must personally prepare and understand any written material you hand in. You may *not* consult with fellow students on exams or on the final project.