

CHEMISTRY 460/562

Physical Chemistry III/Advanced Quantum Chemistry

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Office: LSC 451

Text: Molecular Quantum Mechanics, P.W. Atkins and R.S. Friedman, Fifth ed., Oxford, 2011.

This course provides the student an advanced view of quantum chemistry. All students enrolled should have had at least two semesters of undergraduate physical chemistry, and mathematics through differential equations. Topics not covered by the text will be covered in the lecture, with some references to other sources, including journal articles.

GRADING POLICY

The grading for this course will be based on examination performance (300 points for each semester exam, 400 points for the final exam). Homework problems from the text will be assigned, but not collected. **All in-class exams must be done with non-communicating devices (pencil, pen, slide rule, abacus, noncommunicating calculator). Use of a communicating calculator on an in-class exam will result in a score of 0 on that assignment. The instructor reserves the right to further limit the use of calculators on in-class exams.**

Students with Disabilities

Students with disabilities may be eligible for reasonable academic and non-academic accommodations. Students are required to submit relevant and current documentation of their disability. Students are encouraged to contact the Office of Student Support and Success at disabilityservices@scranton.edu or (570) 941-4038 if they have or think they may have a disability and wish to determine eligibility for any academic accommodations. For non-academic accommodations, students should contact the Office of Equity and Diversity at non-academic-accom@scranton.edu or (570) 941-6645. Students can access accommodate by clicking [here](#).

Writing Center Services

The Writing Center is a resource designed to help students at all academic levels become better writers. It is a safe space where students from any discipline can receive one-on-one feedback on written assignments from well-trained peer consultants who support students in any stage of the writing process. Students can make an appointment through the my.scranton portal: my.scranton.edu >OSSS Card >Writing Center Scheduler.

Academic honesty:

The first time that a student is caught cheating on an exam or is caught plagiarizing he or she will receive a grade of zero points for that assignment. For further consequences of violating academic ethics please refer to the University of Scranton Student Handbook.

<https://www.scranton.edu/academics/cte/acad-integ/acad-code-honesty.shtml>

DATE	LECTURE TOPIC	CHAPTER
1/27	Mechanics/ Introduction to Quantum Mechanics	0,1
2/3	Quantum Mechanics	2
2/10	Rotational Motion/Angular Momentum	3,4
2/17	Atomic Structure	7
2/24	EXAM I	
3/3	Group Theory	5
3/10	Molecular Structure	6
3/24	Molecular Structure	8
3/31	Computational Chemistry	9
4/7	EXAM II	
4/14	Vibration-Rotation Spectroscopy	10
4/23	Vibration-Rotation Spectroscopy	10
4/28	Molecular Electronic Spectroscopy	11
5/5	Photochemistry	11
5/12	FINAL EXAM	

HOMEWORK ASSIGNMENTS

<u>CHAPTER</u>	<u>PROBLEMS</u>
0	1,5-10, 17
1	1,3,5, 7, 12
2	10-15, 26, 27, 33
3	2-4, 17
4	2, 11, 21
5	1-3, 6, 7, 9,15-18
6	3,13
7	5, 8, 11, 18
8	3, 10-16, 19
9	15-18
10	9, 16-18
11	6-8

The SLO Track

In completing this course students should be able to:

1. generate operators for a quantum system and then calculate an observable property of that system using the operators and wavefunctions.
2. determine the energy of the ground state of one-electron atom or ion.
3. predict the ground state of an atom or ion.
4. predict the structure and properties of a molecule using Gaussian.
5. use the point group of a molecule to generate molecular orbitals for that molecule.
6. predict the electronic ground state of a polyatomic molecule.
7. predict spectroscopic parameters from structure calculations and vice-versa.
8. apply symmetry rules to spectroscopic parameters, molecular structure and chemical reactions.

My Reporting Obligations as a Required Reporter

As a faculty member, I am deeply invested in the well-being of each student I teach. I am here to assist you with your work in this course. Additionally, if you come to me with other non-course-related concerns, I will do my best to help. It is important for you to know that all faculty members are required to report incidents of sexual harassment or sexual misconduct involving students. This means that I cannot keep information about sexual harassment or discrimination, sexual assault, sexual exploitation, intimate partner violence or stalking confidential if you share that information with me. I will keep the information as private as I can but am required to bring it to the attention of the University's Title IX Coordinator, Elizabeth M. Garcia, or Deputy Title IX Coordinator, Diana Collins Gilmore, who, in conversation with you, will explain available support, resources, and options. I will not report anything to anybody without first letting you know and discussing choices as to how to proceed. The University's Counseling Center (570-941-7620) is available to you as a confidential resource; counselors (in the counseling center) do not have an obligation to report to the Title IX Coordinator.

Non-Discrimination Statement

The University is committed to providing an educational, residential, and working environment that is free from harassment and discrimination. Members of the University community, applicants for employment or admissions, guests, and visitors have the right to be free from harassment or discrimination based on race, color, creed, religion, ancestry, gender, sex, pregnancy and related conditions, sexual orientation, gender identity or expression, age, disability, genetic information, national origin, ethnicity, family responsibilities, marital status, veteran or military status, citizenship status, or any other status protected by applicable law.

Students who believe they have been subject to harassment or discrimination based on any of the above class of characteristics, or experience sexual harassment, sexual misconduct or gender discrimination should contact Elizabeth M. Garcia, Title IX Coordinator, (570) 941-6645 elizabeth.garcia2@scranton.edu, or Deputy Title IX Coordinators Diana Collins Gilmore (570) 941-6645 diana.collinsgilmore@scranton.edu. The United States Department of Education's Office for Civil Rights (OCR) enforces Title IX. Information regarding OCR may be found at www.ed.gov/about/offices/list/ocr/index.html.