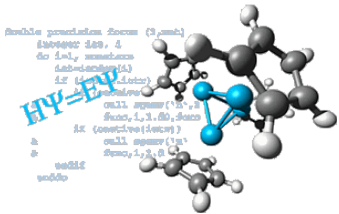# CHEM 161 - Quantum Chemistry

Time: 9:40-10:30 AM MWF

Room: Terrill 207

Lecturer: Jianing Li (jianing.li@uvm.edu, Cook A223)

Office Hour: 10:40-11:30 AM MWF

Summary

CHEM 161 covers quantum mechanics and some of its applications in modern chemistry (e.g. spectroscopy and computation). The goal of this course is to provide students with a fundamental understanding of the quantum chemical description of atoms and molecules. Students will understand the underlying theory of many facts and rules from previous chemistry courses and obtain the background and skills for further courses and researches.
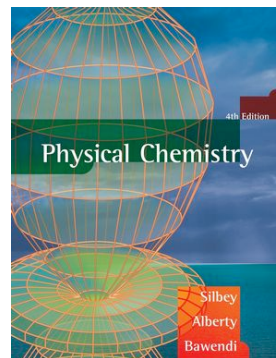
Prerequisites

- PHYS 012, 042, or 152.
- MATH 121 or 124, or the special preparation course CHEM 167 (5:05-6:20 PM MW). Prior knowledge of a math software program (e.g. Mathematica or Matlab) is helpful.

Textbooks

Required:

- Physical Chemistry, 4th Edition, by Silbey, Alberty, and Bawendi (ISBN-13: 978-0471215042)

Other Sources:

- Quantum Chemistry, D.A. McQuarrie
- Quantum Chemistry, I.N. Levine
- Molecular Quantum Chemistry, P. Atkins

Topics

Lecture	Topic	Lecture	Topic
1-4	Background and the Schrödinger Equation	**20-24**	Multi-Electron Atoms
5-8	Particle in the Box	**25-31**	Molecular Bonding
9-14	Harmonic Oscillator and Rigid Rotor	**32-38**	Spectroscopy
15-19	Hydrogen Atom	**39-40**	Modeling with Quantum Chemistry

Note: Lecture numbers are very approximate.

Grading

- 7 in-class quizzes (15%)
- 7 homework assignments (10%)
- 2 midterm exams (40%)
- 1 final exam (35%)

Student Learning Accommodations: In keeping with University policy, any student with a documented disability interested in utilizing accommodations should contact ACCESS, the office of Disability Services on campus. ACCESS works with students and faculty in an interactive process to explore reasonable and appropriate accommodations via an accommodation letter to faculty with recommended accommodations as early as possible each semester.

Contact ACCESS: A170 Living/Learning Center; 802-656-7753; access@uvm.edu; www.uvm.edu/access

UVM's policy on disability certification and student support: www.uvm.edu/~uvmppg/ppg/student/disability.pdf

Religious Holidays: Students have the right to practice the religion of their choice. If you need to miss class to observe a religious holiday, please submit the dates of your absence to me in writing by the end of the second full week of classes. You will be permitted to make up work within a mutually agreed-upon time.

Academic Integrity: The policy addresses plagiarism, fabrication, collusion, and cheating. http://www.uvm.edu/~uvmppg/ppg/student/acadintegrity.pdf

Grade Appeals: If you would like to contest a grade, please follow the procedures outlined in this policy: http://www.uvm.edu/~uvmppg/ppg/student/gradeappeals.pdf

Grading: For information on grading and GPA calculation, go to www.uvm.edu/academics/catalogue and click on Policies for an A-Z listing.

Code of Student Rights and Responsibilities: www.uvm.edu/~uvmppg/ppg/student/studentcode.pdf

FERPA Rights Disclosure: The purpose of this policy is to communicate the rights of students regarding access to, and privacy of their student educational records as provided for in the Family Educational Rights and Privacy Act (FERPA) of 1974. http://www.uvm.edu/~uvmppg/ppg/student/ferpa.pdf

Promoting Health & Safety:
The University of Vermont's number one priority is to support a healthy and safe community:

> *Center for Health and Wellbeing* http://www.uvm.edu/~chwb/
> *Counseling & Psychiatry Services (CAPS)* Phone: (802) 656-3340
> *C.A.R.E.* If you are concerned about a UVM community member or are concerned about a specific event, we encourage you to contact the Dean of Students Office (802-656-3380).   If you would like to remain anonymous, you can report your concerns online by visiting the Dean of Students website at http://www.uvm.edu/~dos/

Final exam policy: The University final exam policy outlines expectations during final exams and explains timing and process of examination period. http://www.uvm.edu/academics/catalogue2013-14/?Page=allpolicies.php&SM=policymenu.html&policy=Exams