



Syllabus

CHM 5580-0001 – Advanced Physical Chemistry

Fall 2017

Lecture Time: Thursday, 6:00 p.m. - 8:50 p.m.

Lecture Location: BA1 O225

Instructor: Dr. Gang Chen

E-mail: Gang.Chen@ucf.edu

Office: Room 201 – Physical Sciences Building

Office Hours: Friday, 2:30 p.m. - 5:30 p.m. or by appointment

Descriptions: As an introduction to Quantum Chemistry and Molecular Spectroscopy, this course will cover the fundamental concepts of quantum mechanics and its application in chemistry. The lectures will follow the primary textbook closely with additional material and concepts drawn from other texts. It starts from the postulates and theorems in quantum mechanics, followed by the electronic structure of atoms, and then the molecule and solid structures. The purpose of this course is to make students understand the chemistry and chemical physics phenomenon from the microstructure of the substance. The course is offered for graduate and advanced undergraduate students in chemistry, physics and engineering.

Primary Textbook: Donald A. McQuarrie, “*Quantum Chemistry*”, 2nd Edition, University Science Books, 2008, ISBN: 978-1-891389-50-4. Good introductory textbook covering most of the topics of this course.

Recommended Textbook: Ira N. Levine, “*Quantum Chemistry*”, 7th Edition, Pearson, 2014, ISBN-13: 978-0-321-80345-0. More mathematical detail included.

Webcourses@UCF: Course materials, grades, related information, and, or announcements, are posted. Please see the posted ones now. Visit daily or as often as possible.

Topics to be covered:

- 1) Historical background of the quantum theory
- 2) Classical wave equation
- 3) Schrodinger equation and a particle in a box
- 4) Postulates and general principles of quantum mechanics
- 5) Harmonic Oscillator and vibrational spectroscopy
- 6) Rigid rotator and rotational spectroscopy
- 7) The Hydrogen atom
- 8) Approximation method, variation theory, perturbation theory
- 9) Many electron atoms
- 10) Chemical bond: one- and two-electron molecules
- 11) Qualitative theory of chemical bonding
- 12) Hartree-Fock-Roothaan method



TENTATIVE SCHEDULE – Fall 2017

Days	Lectures based on...
Aug 24- Sep 14	1) Historical background of the quantum theory 2) Classical wave equation 3) Schrodinger equation and a particle in a box 4) Postulates and general principles of quantum mechanics
Thursday, Sep. 21	Exam 1
Sep 28 - Oct 19	5) Harmonic Oscillator and vibrational spectroscopy 6) Rigid rotator and rotational spectroscopy 7) The Hydrogen atom 8) Approximation method, variation theory, perturbation theory
Thursday, Oct. 26	Exam 2
Nov 2 – Nov 30	9) Many electron atoms 10) Chemical bond: one- and two-electron molecules 11) Qualitative theory of chemical bonding 12) Hartree-Fock-Roothaan method
Thursday, Dec. 7	Final Exam – Cumulative (7:00 p.m. – 9:50 p.m.)

Class Preparations: It is necessary to read the textbook before the lecture and do the homework to reinforce understanding of key principles & concepts, to help develop effective problem solving skills, and to prepare for the exams.

Exams: All exams will be given during regularly scheduled class time. Since the exam dates are given well in advance, there will be no make-up exams except in the case of illness. A written notice in advance and a doctor's exemption will be required and a make-up exam could be administrated.

Calculator Policy: Only basic and scientific calculators (without graphic functions) are allowed for all exams in class (e.g., TI-30XA). **NO GRAPHING CALCULATORS ARE ALLOWED!!!** Any use of electronic device (iPod, cell phone, MP3 player, computer...) during exams is strictly prohibited. Any use of such device will be considered an attempt to cheat on the exam and will result in a 0 on the grade.

Homework: There will be 10 assigned problem sets which will be handed out on Thursday after class and will be due in a week before the class. The solutions will be posted on the webcourses after the due day. Homework received late will automatically be deducted 50%.

Extra credit: Randomly distributed in class.



Grading:

2 In-course Exams (each 150 pts)	300 pts
Final Exam (cumulative)	200 pts
10 homework (each 35 pts)	350 pts
Class performance (each 10 pts)	150 pts
Grand Total	1000 pts

The final grade will be calculated on the basis of the total points.

950 - 1000	= A
900 - 949	= A-
850 - 899	= B+
800 - 849	= B
750 - 799	= B-
700 - 749	= C+
650 - 699	= C
600 - 649	= C-
500 - 599	= D
< 500	= F

Academic Integrity

Academic integrity is at the center of the educational experience at UCF. Therefore students are expected to uphold the highest standards of academic integrity and not engage in nor tolerate academic dishonesty. Academic dishonesty includes, but is not limited to, fabrication, cheating or plagiarism. Any violation of academic integrity will be investigated and, where warranted, the student will receive appropriate sanctions through the University's Student Conduct Process. *Please familiarize yourself with the current UCF Student Handbook.* In particular, adherence to the Student Conduct Policy and Academic Integrity Policy will help to ensure that your learning and living experiences are founded on integrity.

Classroom Conduct

Disruptive behavior is not tolerated. The instructor will consult with students consistently interrupting classroom routine. Students are subject to removal from class permanently. Cell phones and pagers must be on silent mode during class and tests. Laptop computers are allowed for note taking purposes only. **No audio or video recording is allowed without the instructor's authorization.**

Accommodations for the differently-able students

Students with disabilities who qualify for academic accommodations must present a letter from the office of Students Accessibility Services (SAS) and discuss specific needs with the instructor, preferably within the first two weeks of class. The SAS determines accommodations based on appropriate documentation of disabilities (Ferrell Commons, Room 185, 407/823-2371).

In the best interest of fulfilling the course objectives and assuring the academic integrity of the institution, the instructor reserves the right to modify/change any part of this schedule/syllabus if warranted!

Recipe for Success in CHM 5580

* **Attend every class** - You will find that students, who attend every class, listen to the instructor and take good notes will be more likely to pass with a higher grade. If you have an



emergency or illness, contact your instructor ahead of time to let her/him know that you will be absent. A local study showed that students who missed the first class meeting were more likely later to withdraw or fail. Important note: if you miss a class it is your responsibility to meet with the instructor, outside of regular class time, to determine a plan to make up the missed work.

* **Do not lobby/negotiate for a grade!**

* **Understanding** - the various concepts are vital to learn chemistry. Memorizing is a recipe for disaster!

* **Review lecture material early and often** - Do not wait until the last few minutes before a test to do the necessary revision.

* **Review the worked *exercises/examples* in the textbook** - Also at the end of each chapter is a list of chapter goals. Those serve as helpful review tools. Find time to work on the suggested end-of-chapter problems. Practice makes perfection.

* **The instructor strongly encourages you to use office hours for discussing the material covered in classes and reviewing exams** - Get assistance ASAP, if needed. Please make use of the Student Academic Resource Center (SARC); Howard Phillips Hall 113; www.sarc.sdes.ucf.edu.

* **When having academic difficulty seek assistance** - Your instructor is always willing to assist you however, there are other ways to get help. The Student Academic Resource Center (SARC) has Peer Tutoring and SI Leaders - undergraduate students who have already taken and succeeded in the course). The Department of Chemistry offers free one-on-one tutoring sessions with a chemistry graduate student at the Chem.