

INSTRUCTOR: Dr. Eugene Wagner

OFFICE: Chevron 107 & Thaw 400

OFFICE HOURS: see website

PHONE: 624-2861

E-MAIL: ewagner@pitt.edu - This is the best way to reach me.

CLASS WEBSITE: <http://chemicaleducation.org> Always refer to the site for updated information.

TEXTBOOK: *Physical Chemistry 2nd ed.*, by David Ball

OBJECTIVES OF COURSE: The primary purpose of this course is to increase your understanding of Physical Chemistry concepts and applications. Through this course you should gain an appreciation for the fundamental chemical principles that ultimately control and determine macroscopic physical and chemical properties. The most important attributes that you must bring to this course are an enthusiasm for learning and an open mind.

ATTENDANCE POLICY: Attendance at all lectures is very important. While we will have a very good textbook to help convey the information of this course, the emphasis of specific material and topics will be conveyed through the lectures. You will be responsible for all material and concepts covered in the lectures, assigned readings, textbook, and homework sets. **If you miss a graded assignment, you will receive a zero for that assignment. There are no make-ups for assignments.**

DISABILITY SERVICES: If you have a disability for which you are or may be requesting an accommodation, you are encouraged to contact me and the Office of Disability Resources and Services, 216 William Pitt Union, (412) 6487890/(412) 383-7355 (TTY) as early as possible in the term. DRS will verify your disability and determine reasonable accommodations for this course.

ACADEMIC HONESTY: Students are responsible for knowing and observing the University of Pittsburgh Code of Student Academic Integrity, which forbids cheating, fabrication or falsification of information, multiple submissions of academic work, plagiarism, abuse of academic materials, and complicity in academic dishonesty. Academic evaluation in this course includes a judgment that the student's work is free from dishonesty. Students who are suspected of violating this code will be required to participate in the legal procedural process as outlined in the University Guidelines on Academic Integrity.

CODE OF CONDUCT AND PROFESSIONALISM: You will be required to always conduct yourself in a professional and courteous manner toward the professor and all students in the class. Failure to do so will result in loss of points for the class and the potential for removal from the course.

TOPICS TO BE COVERED: (subject to change) see class website for details
Quantum Mechanics, Molecular Orbital Theory, Molecular Modeling, Statistical Thermodynamics

EXAMS: The tentative schedule is as follows:

EXAM 1	02/06/16	Quantum Mechanics - The Basics
EXAM 2	03/20/16	Quantum Mechanics - Real Systems
EXAM 3	04/03/16	Computational/Molecular Modeling - in class portion (40%) Computational project (60%) - see website
EXAM 4	Final Exam Week	Statistical Thermodynamics

HOMEWORK: Homework assignments will be listed on the course website. You will be accountable on exams for the content and concepts introduced and exemplified in these homework problems. Homework will be collected for a grade. All graded HW combined together will count as one Exam.

GRADING SCALE: There is no absolute grading scale for this course. However, estimated exam letter grades will be disseminated after each exam. Exams and your total HW score are each worth 20% of your total score for the course.

Tentative Lecture Schedule for Chem1480, Spring 2017

Week	Date	Lecture	Homework and Resources from Lecture
1	1/2	No Class	
	1/4	Quantum Mechanics: Fundamental Discoveries Start reading Chapter 9	Lecture Slides HW: Science-Engineering interface essay, due 1-9-17. See Lecture slides for details
2	1/9	Quantum Mechanics: Fundamental Discoveries Read Chapter 9	Lecture 2 Slides Development of Quantum Mechanics QMHW1: Quantum assignment 1 – Due Tuesday, 1/17 by noon. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
	1/11	QM: Waves Start reading Chapter 10	Lecture 3 Slides
3	1/16	No Class	
	1/18	QM: Operators, Eigen Values	Lecture 4 Slides QMHW2: Quantum assignment 2 – Due Thursday, 1/26 by 4pm. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
4	1/23	QM: Probability, Normalization, PIB Read chapter 10 through section 10.	Lecture 5 Slides
	1/25	QM: PIB, Conductors	Lecture 6 Slides
5	1/30	QM: STM, Expectation values, 3-D PIB, Degeneracy, Orthogonality Chapter 10, sec. 11-13	Lecture 7 Slides QMHW3: Quantum assignment 3 – Due Friday, 2/3 by 4pm. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
	2/1	QM: Vibrational Energy Chapter 11, sec. 1-5	Lecture 8 Slides
6	2/6	QM: Vibrational Energy, IR spectra Chapter 14, sec. 8-12 as it relates to lecture. Q&A for Exam	Lecture 9 Slides QMHW4: Quantum assignment 4 – Due Monday, 2/20 by 4pm. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
	2/8	Exam 1: The Basics of Quantum Mechanics Infosheet supplied with exam. A Periodic Table is also provided Answer Key Regrades for the exam must be submitted in writing (just put a note on the front page with the specific questions). Any exam submitted for regrade will have the entire grading of the exam reviewed and revised as needed.	
7	2/13	QM: IR spectra, 2-D Rotation Chapter 11, sec. 6-8	Lecture 10 Slides
	2/15	QM: 3-D Spherical Coordinates, Rotational spectra Chapter 14, sec. 4-7 as it relates to lecture.	Lecture 11 Slides
8	2/20	QM: The Hydrogen Atom Chapter 11, sec. 9-12	Lecture 12 Slides QMHW5: Quantum assignment 5 – Due Friday, 3/3 by noon. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
	2/22	QM: Perturbation and Variation Theories Read chapter 12, but follow lecture notes closely	Lecture 13 Slides
9	2/27	QM: Variation Theory, LCAO-MO Read chapter 12, but follow lecture notes closely	Lecture 14 Slides
	3/1	QM: LCAO-MO, Huckel Method	Lecture 15 Slides QMHW6: Quantum assignment 6 – Due Friday, 3/17 by noon. Hand in

		Read chapter 15 in our book (sec. 9&10)	to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
10	3/6	NO CLASS! SPRING BREAK!!!	
	3/8	NO CLASS! SPRING BREAK!!!	
11	3/13	QM: Huckel Method Read chapter 15 in our book (sec. 9&10)	Lecture 16 Slides
	3/15	QM: Huckel Method Read chapter 15 in our book (sec. 9&10)	Lecture 17 Slides
12	3/20	Exam 2: Quantum Mechanics of Real Systems Infosheet supplied with exam. A Periodic Table is also provided Answer Key	
	3/22	Computational Methods: Basis Sets, Methods, Energy Optimization, Electron Densities	Installing and start up of Scigress Engel-ComputationalChemistry.pdf (18Mb)-Comprehensive coverage of topic MMWorkbook.pdf (5Mb) - supportive information about orbital presentations and views in molecular modeling Excel File for CCLab 2
13	3/27	Computational Methods: Spectroscopy, Thermochemistry, Transition States, Protein Studies	Labs 1,2,3 due. Hand in to mailboxes labeled "Lab 1, 1480", "Lab 2, 1480", "Lab 3, 1480". Lab 2 can be handed in by Wednesday with no late penalty, but try to get it completed by today so that you do not fall behind with these assignments.
	3/29	Statistical Thermodynamics Chapter 17, all sections	Labs 4-5 due. Hand in to mailboxes labeled "Lab 4, 1480", "Lab 5, 1480" in hallway outside of room 107. Labs 6-8 due. Hand in to mailboxes labeled "Lab 6, 1480", "Lab 7, 1480", and "Lab 8, 1480" in hallway outside of room 107.
14	4/3	Statistical Thermodynamics Chapter 17, all sections	STHW1: Stat Thermo HW1 – Due 4/12 by class time. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. Answer Key
	4/5	Exam 3: Computational Methods in class portion AnswerKey	Final due date for all Molecular Modeling labs. No labs will be accepted after this date. Questions presented in lecture Molecular Modeling Project Grading Rubric (due date: 4/19) Project ideas - Be sure to talk with Dr. Wagner if you have questions about selecting a project idea.
15	4/10	Statistical Thermodynamics Chapter 17, all sections	
	4/12	Statistical Thermodynamics Chapter 17, all sections	Lecture slides STHW2: Stat Thermo HW2 – Due 4/19 by class time. Hand in to mailbox labeled "Chem 1480" in hallway outside of room 107. NOT all problems are graded. Hand in problems 1-6. The others are for your reference. Answer Key
16	4/17	Statistical Thermodynamics Chapter 18, sections 1-9	Lecture slides
	4/19	Statistical Thermodynamics Chapter 18, sections 1-9	Lecture slides Molecular Modeling Project Due today- Turn in at class. Make sure to staple the grading rubric to the front and include your names.
17	Monday 4/24 at 10 am	Exam 4: Statistical Thermodynamics Infosheet supplied with exam. A Periodic Table is also provided	