CHM5440 - Physical Chemistry II

Winter 2015

H. Bernhard Schlegel	375 Chemistry
e-mail: <u>hbs@chem.wayne.edu</u>	(313) 577-2562
G. Andrés Cisneros	333 Chemistry
e-mail: andres@chem.wayne.edu	(313) 577-2571
	H. Bernhard Schlegele-mail: <u>hbs@chem.wayne.edu</u>G. Andrés Cisnerose-mail: <u>andres@chem.wayne.edu</u>

Lectures: Mon, Wed 12:50-2:40 PM, 312 State Hall

Office Hours: Thursday 2-3 PM. We will be readily available for after-class questions or discussions or make appointments by asking after class or by e-mail. Please include **CHM5440** in the subject line

Required Text: Physical Chemistry, by R. J. Silbey, R. A. Alberty, and M. G. Bawendi, 4th Edition (John Wiley & Sons, 2005).

Learning outcomes: At the completion of this course, students should understand the fundamentals of Quantum mechanics and its application to understanding atomic structure, molecular structure and bonding, rotational and vibrational spectroscopy; electronic spectroscopy; the kinetic theory of gases; and the elements of chemical kinetics The emphasis will be on the *fundamental physical principles* that form a unified base for understanding chemistry and spectroscopy.

The first part of the course will be taught by Prof. Cisneros and the second by Prof. Schlegel

• Class work will consist of lectures, group activities and discussion. Attendance and participation is required.

• The reading assignments must be completed BEFORE each lecture.

• There will be regular brief quizzes ($\sim 10 \text{ min}$) quizzes during each lecture that will contribute to the final grade.

- The last day to drop the class is Friday Jan 17, 2014.
- There will be 2 midterm exams (1 hr each) and a final exam (2.5 hrs).
- ◆ In general, exams and quizzes will be closed-book.
- ♦ All exam dates are *final*, permission to miss an exam (with legitimate excuse) must be obtained *24 hours before* the date and time of the exam.
- All homework assignments must be turned in on time, due dates will be announced.

◆ Zero grade (0 pts) will be assigned if an exam/quiz is missed or a homework is not turned in on time.

• Assignments and additional material will be found on Blackboard. It must be checked frequently.

• You can work in groups for homework but you should fully understand the procedure and submit your own write-ups.

 ◆ Grading: Homework: 10% Quizzes: 15% Midterm exams: 50% Final exam: 25%

Grading Scale 100 A 93 A- 88 B+ 84 B 80 B- 77 C+ 73 C 69 C- 66 D+ 63 D 60 D- 55 F

CHM 5440 Tentative Course syllabus:

Week	Date	Topics	Reading
			assignments
1	1/12	Introduction to the course.	
		Math review	
	1/14	Classical mechanics: a deterministic theory. Failures of classical	9.1
		mechanics.	
		The wave-particle duality. The de Broglie wavelength. The	9.1 - 9.3
		Heisenberg Uncertainty Principle. The wavefunction.	
2	1/19	MLK Day, NO CLASS	
	1/21	The Schrödinger equation.	
		Particle in a 1D box: quantization of energy	9.14, 9.3
3	1/26	Operators. Postulates of Quantum Mechanics	9.6
		Particle in 2D and 3D box: <i>degeneracy</i>	9.4, 9.5, 9.13
		Last day to drop class (1/27)	
	1/28	Tunneling	9.7
		Vibrational motion: Harmonic Oscillator	9.15
4	2/2	Quantum-mechanical Harmonic Oscillator	9.9
		Commutator and the uncertainty principle. The superposition	9.10
		principle.	
	2/4	Rotational motion: classical description	9.4, 9.5, 9.8
		Rotational motion in 2D: particle on a ring.	9.11
5	2/9	Review; Exam I	
	2/11	Rotational motion in 3D. Angular momentum.	9.11, 9.12
		Hydrogen atom: the Schrodinger equation	10.1, 10.15
6	2/16	Hydrogen atom: energy levels, spectra	10.1, 10.2
		Hydrogen atom: wavefunctions	10.3
	2/18	Hydrogen atom: expectation values of physical observables.	10.3, 10.4
		Variational Method	10.6
7	2/23	Helium Atom	10.7
		Electron spin. Pauli Exclusion Principle	10.5, 10.8
	2/25	Multi-electron atoms: the Aufbau Principle and the periodic table	10.10, 10.11
		Atomic spectroscopy	10.12, 10.13

8	3/2	Atomic spectroscopy	10.13, 10.14
		Quantum Chemistry. The SCF Hatree-Fock Method	10.9
	3/4	Diatomic molecules: the Born-Oppenheimer Approximation	11.1
		The hydrogen molecular ion H_2^+	11.2
9	3/9	MO description of the hydrogen molecule	11.3,11.4
	3/11	Electron configuration of homonuclear diatomics	11.5
	3/16	Spring Break	
	3/18	Spring Break	
10	3/23	Polyatomic molecules: Valence bond method	11.6
		Polyatomic molecules: Huckel MO theory	11.7
		The band theory of solids: metals, semiconductors, inculators	11.11
	3/25	Spectroscopy: an introduction	13.1, 13.2
		Rotational spectra of diatomics	13.3, 13.4
11	3/30	Vibrational spectra of diatomics	13.6
		Vibration-rotation spectra	13.7
	4/1	Vibrations of polyatomic molecules	13.8
		Electronic spectroscopy of diatomics	14.1 - 14.4
12	4/6	Electronic spectroscopy of diatomics	14.3, 14.5
		Photochemistry and chemical dynamics	14.8, 19.10
	4/8	Kinetic theory of gases: the Maxwell distribution, Review	17.1 - 17.3
		Exam II	
13	4/13	Collisions of the gas-phase molecules. Pressure. Mean free path	17.5 - 17.8
		Transport phenomena: diffusion and viscosity.	17.10, 17.11
	4/15	Chemical kinetics: reaction rates	18.1, 18.2
		Order of reactions.	18.2
14	4/20	Reversible reactions and the detailed balance principle	18.3, 18.5,
			18.8
		Consecutive reactions and kinetic schemes	18.4
	4/22	Reaction mechanisms	18.7
		Temperature dependence of the reaction rates	18.6
15	4/27	Bimolecular reactions. <i>Final Review</i>	18.9,18.11,
			18.12
		Final Exam (date and time TBA)	

General Notes

Religious Holidays

Because of the extraordinary variety of religious affiliations of the University student body and staff, the Academic Calendar makes no provisions for religious holidays. However, it is University policy to respect the faith and religious obligations of the individual. Students with classes or examinations that conflict with their religious observances are expected to notify their instructors well in advance so that mutually agreeable alternatives may be worked out.

Student Disabilities Services

If you have a documented disability that requires accommodations, you will need to register with Student Disability Services for coordination of your academic accommodations. The Student Disability Services (SDS) office is located in the Adamany Undergraduate Library. The SDS telephone number is 313-577-1851 or 313-202-4216 (Videophone use only). Once your accommodation is in place, someone can meet with you privately to discuss your special needs. Student Disability Services' mission is to assist the university in creating an accessible community where students with disabilities have an equal opportunity to fully participate in their educational experience at Wayne State University.

Students who are registered with Student Disability Services and who are eligible for alternate testing accommodations such as extended test time and/or a distractionreduced environment should present the required test permit to the professor at least one week in advance of the exam. Federal law requires that a student registered with SDS is entitled to the reasonable accommodations specified in the student's accommodation letter, which might include allowing the student to take the final exam on a day different than the rest of the class.

Academic Dishonesty -- Plagiarism and Cheating

Academic misbehavior means any activity that tends to compromise the academic integrity of the institution or subvert the education process. All forms of academic misbehavior are prohibited at Wayne State University, as outlined in the Student Code of Conduct (http://www.doso.wayne.edu/student-conduct-services.html). Students who commit or assist in committing dishonest acts are subject to **downgrading** (to a failing grade for the test, paper, or other course-related activity in question, or for the entire course) and/or **additional sanctions** as described in the Student Code of Conduct.

Cheating: Intentionally using or attempting to use, or intentionally providing or attempting to provide, unauthorized materials, information or assistance in any academic exercise. Examples include: (a) copying from another student's test paper; (b) allowing another student to copy from a test paper; (c) using unauthorized material such as a "cheat sheet" during an exam.

Fabrication: Intentional and unauthorized falsification of any information or citation. Examples include: (a) citation of information not taken from the source indicated; (b) listing sources in a bibliography not used in a research paper.

Plagiarism: To take and use another's words or ideas as one's own. Examples include: (a) failure to use appropriate referencing when using the words or ideas of other persons; (b) altering the language, paraphrasing, omitting, rearranging, or forming new combinations of words in an attempt to make the thoughts of another appear as your own.

Other forms of academic misbehavior include, but are not limited to: (a) unauthorized use of resources, or any attempt to limit another student's access to educational resources, or any attempt to alter equipment so as to lead to an incorrect answer for subsequent users; (b) enlisting the assistance of a substitute in the taking of examinations; (c) violating course rules as defined in the course syllabus or other written information provided to the student; (d) selling, buying or stealing all or part of an unadministered test or answers to the test; (e) changing or altering a grade on a test or other academic grade records.

Course Drops and Withdrawals In the first two weeks of the (full) term, students can drop this class and receive 100% tuition and course fee cancellation. After the end of the second week there is no tuition or fee cancellation. Students who wish to withdraw from the class can initiate a withdrawal request on Pipeline. You will receive a transcript notation of WP (passing), WF (failing), or WN (no graded work) at the time of withdrawal. No withdrawals can be initiated after the end of the tenth week. Students enrolled in the 10th week and beyond will receive a grade. Because withdrawing from courses may have negative academic and financial consequences, students considering course withdrawal should make sure they fully understand all the consequences before taking this step. More information on this can be found at:

http://reg.wayne.edu/pdf-policies/students.pdf

Student services

The Academic Success Center (1600 UndergraduateLibrary) assists students with content in select courses and in strengthening study skills. Visit www.success.wayne.edu for schedules and information on study skills workshops, tutoring and supplemental instruction (primarily in 1000 and 2000 level courses).