Chemistry 3412: Physical Chemistry II

Instructor:

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Requirements and Grading Scheme:

Problem sets	15%
Three tests	60%
Final	25%

Auditors are required to take the final exam and score at least 20%. Pass/Fail students must take all three tests and the final and receive an overall passing grade. Auditors and Pass/Fail students are not required to do problem sets but may turn them in for extra credit.

Honor Code

Any student caught plagiarizing will be dealt with according to policies outlined in the GT Academic Honor Code. As noted in the Honor Code website (`http://www.honor.gatech.edu`), plagiarizing is defined by Webster's as, "to steal and pass off (the ideas or words of another) as one's own : use (another's production) without crediting the source." For this class, you may not use anyone else's words or work as if they were your own. You may not copy any part of any assignment from other students, previous students, or any other sources. You are encouraged to show all of your work on assignments, as failure to do so may raise suspicions that you have copied the work of others without understanding it. You may discuss homeworks/problem sets with other students, but you must write up the solutions on your own without consulting written solutions from any source. This policy is for your own protection; in the past, students who relied on others for problem set solutions were not prepared to pass the tests.

Course Website:

We will use the T-square website for handouts, announcements, etc.

Lecture Schedule:

The tentative lecture schedule is given in the table below. The latest version may be found on the course website. *Key dates such as drop day and holidays are subject to change by Georgia Tech. Please check the official academic calendar.*

Textbook: D. A. McQuarrie, *Quantum Chemistry* (2nd edition), University Science Books, Sausalito, CA, 2008. *If you have Physical Chemistry by McQuarrie and Simon, you do not need an additional book; the textbook is contained within the larger McQuarrie and Simon book.* Handouts will be given for the statistical mechanics material, but you may wish to consult N. O. Smith, *Elementary Statistical Thermodynamics: A Problems Approach*, Plenum Press, New York, 1982.

Date	Topic	Reading
1/11	Scope and Philosophy of Quantum Mechanics, Course Outline, Applications of Quantum Mechanics	
1/13	Historical first steps towards QM: UV catastrophe, Photoelectric effect, H atom spectrum, quantization, Bohr model	1-25
1/15	Wave-particle duality, interpretation of Bohr model, uncertainty principle	26-36
1/18	School Holiday	
1/20	Waves and the Classical Wave Equation	53-72
1/22	The Schrödinger Equation (time-independent and time-dependent)	97-105
1/25	Particle in a box, Free particle	105-119
1/27	3D Systems. Separability of coordinates, 3D particle in a box	114-119
1/29	Operators and Commutators	153-155,156-165 Handout
2/1	Uncertainty Principles	155-156
2/3	**Test I**	
2/5	Postulates of Quantum Mechanics	143-170
2/8	Superpositions of States	170-175
2/10	Harmonic Oscillator I: Classical HO	207-215
2/12	Harmonic Oscillator II: Quantum HO	215-219, 225-228
2/15	Harmonic Oscillator III: Properties of HO wavefunctions	228-233
2/17	Harmonic Oscillator IV: Vibrational spectra, Polyatomics	219-224, 233-239
2/19	Rigid Rotor, Spherical Harmonics	255-275, 282-290
2/22	Angular Momentum	290-300
2/24	Vibrational-Rotational Spectra I	275-281
2/26	Vibrational-Rotational Spectra II: Higher-order terms	281-282
2/29	**Test II**	
3/2	Hydrogen Atom I	321-327
3/4	Hydrogen Atom II	327-360

3/7	Approx. Methods I: Perturbation Theory	396-410
3/9	Approx. Methods II: Variational Methods	381-387
3/11	Linear Variation Method and Secular Determinants	387-396
3/14	Atoms I. Atomic Hamiltonian, Atomic units	435-444
3/16	Intro to Hartree-Fock method, Slater determinants	444-458
3/18	Hartree-Fock method and electron correlation	458-466
3/21-3/25	Spring Break	
3/28	Atoms II. Electron configurations and term symbols, Aufbau principle	466-474, Handout
3/30	Atoms III. Hund's rules, Spin-orbit effects	474-482
4/1	**Test III**	
4/4	Molecules. Born-Oppenheimer Approximation, LCAO-MO treatment of H_2^+	499-515
4/6	Hartree-Fock and CI for H_2	521-543
4/8	Diatomics: Molecular orbitals, term symbols	559-581, Handout
4/11	Diatomics II	
4/13	Computational Quantum Chemistry	607-653
4/15	Introduction to Group Theory	Handout
4/18	Introduction to Statistical Mechanics Scope, Ensemble averages, Goals	Smith Ch. 1 Atkins Ch. 19
4/20	Canonical ensemble, Boltzmann distribution, Ensemble partition functions	Smith Ch. 1 Atkins Ch. 19
4/22	Partition functions for indistinguishable particles and thermo properties (e.g., E, S, C_v, H, A, G)	Smith Ch. 4 Atkins Ch. 20
4/25	Molecular partition functions, ideal gas law from stat mech + particle in a box	Smith Ch. 4 Atkins Ch. 20