

Chemistry 3412: Physical Chemistry II

Instructor:

Instructor: Professor David Sherrill
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Office: MS&E 2100N
Office Hours: MW 2-3 or by appointment

Requirements and Grading Scheme:

Problem sets	10%
Three tests	60%
Final	30%

Auditors are required to take at least three of the four exams (3 tests + final) and demonstrate at least a minimal knowledge of the subject. 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:

A course website will be available with the latest version of the syllabus, handouts, etc. Look under under <http://vergil.chemistry.gatech.edu/courses/chem3412/>. I will also try to keep the T-square site up to date.

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.*

TA: James Bradshaw

Textbook: D. A. McQuarrie, *Quantum Chemistry*, University Science Books, Mill Valley, CA, 1983. *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
8/20	Scope and Philosophy of Quantum Mechanics, Course Outline, Applications of Quantum Mechanics	
8/22	Historical first steps towards QM: UV catastrophe, Photoelectric effect, H atom spectrum, quantization, Bohr model	3-30
8/24	Wave-particle duality, interpretation of Bohr model, uncertainty principle	30-39
8/27	Waves and the Classical Wave Equation	47-64
8/29	The Schrödinger Equation (time-independent and time-dependent)	77-85, 120-123
8/31	Particle in a box, Free particle	85-101
9/3	Labor Day (School Holiday)	
9/5	Operators and Commutators	126-133,135-140 Handout
9/7	Uncertainty Principles	
9/10	Test I	
9/12	Postulates of Quantum Mechanics	113-125
9/14	Superpositions of States	120-123,133-135
9/17	Harmonic Oscillator I: Classical HO	153-162
9/19	Harmonic Oscillator II: Quantum HO	175-180, Mz. 53-61
9/21	Harmonic Oscillator III: Properties of HO wavefunctions	163-184
9/24	Harmonic Oscillator IV: Vibrational spectra	163-165
9/26	3D Systems. Separability of coordinates, 3D particle in a box	195-206
9/28	Rigid Rotor, Spherical Harmonics	206-217
10/1	Angular Momentum	217-221, Mz. 187-190
10/3	Test II	
10/5	Vibrational-Rotational Spectra I	437-449
10/8	Fall Break	
10/10	Vibrational-Rotational Spectra II: Higher-order terms	449-460
10/12	Hydrogen Atom I	221-225
10/15	Hydrogen Atom II	225-242

10/17	Approx. Methods I: Perturbation Theory	242-243, 255-262
10/19	Approx. Methods II: Variational Methods	262-276
10/22	Linear Variation Method and Secular Determinants	
10/24	Atoms I. Atomic Hamiltonian, Atomic units	287-294
10/26	Intro to Hartree-Fock method, spin	295-301
10/29	Antisymmetry, Slater Determinants	301-313
10/31	Atoms II. Electron configurations and term symbols, Aufbau principle	313-326, Handout
11/2	Atoms III. Hund's rules, Spin-orbit effects	319-329
11/5	Molecules. Born-Oppenheimer Approximation, Valence-bond theory	343-358
11/7	LCAO MO Treatment of H_2^+	358-369
11/9	Diatomics: Molecular orbitals, term symbols	369-390, Handout
11/12	Diatomics II	
11/14	Polyatomics: Hybrid orbitals, term symbols	396-409, 457-460
11/16	Test III	
11/19	Introduction to Group Theory	Handout
11/21	Electronic Spectra	460-484
11/23	Thanksgiving break	
11/26	Introduction to Statistical Mechanics Scope, Ensemble averages, Goals	Smith Ch. 1 Atkins Ch. 19
11/28	Canonical ensemble, Boltzmann distribution, Ensemble partition functions	Smith Ch. 1 Atkins Ch. 19
11/30	Partition functions for indistinguishable particles and thermo properties (e.g., E , S , C_v , H , A , G)	Smith Ch. 4 Atkins Ch. 20
12/3	Molecular partition functions, ideal gas law from stat mech + particle in a box	Smith Ch. 4 Atkins Ch. 20
12/5	Quantum contributions to partition functions and thermo properties	Smith Ch. 5 Atkins Ch. 20
12/7	Finish and Review	
