Chemistry 311, Physical Chemistry I **Fall 2011**
University of New Mexico **Dr. H. Guo**

Lectures: 2:00 – 2:50 pm, MWF, Clark 101
Discussions: 3:00 – 3:50 pm, M, Clark 101
Office hours: 12:30-1:30 pm, MWF, Bandelier East 108.

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Syllabus

The microscopic world at the atomic level (i.e. chemistry) is governed by quantum mechanical laws, which are quite different from classical mechanics that dictate our macroscopic world. To understand the structure of molecules and their reactivity, one has no choice but to rely on quantum mechanics. In this course, we will introduce quantum mechanical principles and their applications to atomic and molecular systems. We will start by discussing the failures of classical physics, and the birth of quantum mechanics. Then, basic quantum mechanical concepts such as wave function and its statistical interpretation, eigenvalues and eigenfunctions of quantum operators, the superposition principle, and the uncertainty principle will be introduced. This is followed by analytical solutions of the Schrödinger equation for simple systems, such as the particle in a box, harmonic oscillator, and rigid rotor. These examples not only illustrate energy quantization of microscopic systems, but also have important practical significance as discussed later. We will also show that the application of quantum mechanics to atoms yields naturally the familiar concepts of atomic orbitals and quantized energy levels, which form the bases for a quantum mechanical description of molecular structure discussed in subsequent chapters. Molecular symmetry will then be discussed. Finally, we discuss spectroscopy, which serve as a bridge between the microscopic and macroscopic worlds.

The topics in this class are considered as the most difficult in the Chemistry Curriculum. As a result, students are advised to read the book before the lectures, and follow up with reading and homework. Apart from the lectures, there will be a discussion section on every Monday (3-4 pm), in which the TA will help you with the problems arising from the homework and lectures. Please plan to attend these sessions. In addition, I have allocated one hour on MWF before the lectures to answer questions in my office. Useful information will also be posted at my webpage (www.unm.edu/~hguo)

Homework will be assigned on weekly basis. There will be three midterm exams and a final exam. The final grade will be judged based on the homework (10%), the three midterm exams (20% each), and the final exam (30%). The midterm exams will be held on Sept. 16th, Oct. 12th, and Nov. 11th. The final exam will be on Dec. 14th, 3:00 - 5:00 pm at Clark 101. Make sure your travel schedule does not conflict with the exams. *There will be no makeup exams, except for extraordinary cases.* If you miss one midterm exam the other exams will be weighted more heavily in computing your grade. If you miss all midterm exams or the final exam you will receive a grade of zero for that exam.

The lecture will be based on Physical Chemistry, Ninth Edition, by Peter Atkins and Julio de Paula, W. H. Freeman and Company, Chapters 7- 13.

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Week	Date	Lecture	Topic	Chapter
1	8/22	1	Introduction, classical physics	7
	8/24	2	Blackbody radiation and Planck's distribution	7
	8/26	3	Photoelectric effect, heat capacity, Einstein theories	7
2	8/29	4	Atomic spectra and Bohr's model	7
	8/31	5	Matter-wave duality and de Broglie wave	7
	9/2	6	Quantum operators, Schrödinger equation	7
3	9/5	--	--Labor Day--	--
	9/7	7	Wavefunction, expectation values	7
	9/9	8	Particle in a box, energies	8
4	9/12	9	Particle in a box, wavefunctions	8
	9/14	10	Review	--
	9/16	11	**Exam I**	--
5	9/19	12	Particle in a 2D box, degeneracy	8
	9/21	13	Harmonic oscillator, energies	8
	9/23	14	Harmonic oscillator, properties	8
6	9/26	15	2D rigid rotor, angular momentum	8
	9/28	16	3D rigid rotor, spherical harmonics	8
	9/30	17	Vector model, spin	8
7	10/3	18	Hydrogen atom, solution of Schrödinger equation	9
	10/5	19	Hydrogen atom, quantum numbers	9
	10/7	20	Hydrogen atom, atomic orbitals	9
8	10/10	21	Review	--
	10/12	22	**Exam II**	--
	10/14	--	--Fall Break--	--
9	10/17	23	Multielectron atoms, orbital approximation	9
	10/19	24	Building-up principles	9
	10/21	25	Term symbols, atomic spectra	9
10	10/24	26	Born-Oppenheimer approximation	10
	10/26	27	Hydrogen molecular ion, LCAO-MO	10
	10/28	28	Homonuclear diatoms	10
11	10/31	29	Polyatomic systems, Welsh diagram	10
	11/2	30	Hückel approximation	10
	11/4	31	Symmetry elements	11
12	11/7	32	Symmetry groups	11
	11/9	33	Review	--
	11/11	34	**Exam III**	--
13	11/14	35	Representation and character tables	11
	11/16	36	Applications of group theory	11
	11/18	37	General features of spectroscopy	12
14	11/21	38	Transition rates	12
	11/23	39	Rotational spectroscopy	12
	11/25	--	--Thanksgiving--	--
15	11/28	40	Rotational Raman spectra	12
	11/30	41	Harmonic oscillator and vibrational spectra	12
	12/2	42	Vibration of polyatomic molecules, normal modes	12
16	12/5	43	Electronic transitions, Franck-Condon factors	13
	12/7	44	Lasers and applications	13
	12/9	45	Review	--