Chemistry 311, Physical Chemistry I **Fall 2014**
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. 12th, Oct. 8th, and Nov. 7th. The final exam will be on Dec. 10th (Wednesday), 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 any exam without permission, you will receive a grade of zero for that exam.

The lecture will be based on Quantum Chemistry, Third Edition, by Thomas Engel, Pearson. The homework will be assigned using Mastering Chemistry.

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Week	Date	Lecture	Topic	Chapter
1	8/18	1	Blackbody radiation and photoelectric effect	1
	8/20	2	Matter-wave duality and de Broglie wave	1
	8/22	3	Bohr's atomic model	1
2	8/25	4	Schrödinger equation	2
	8/27	5	Quantum operators, observables	2
	8/29	6	Statistical interpretation of wave functions	3
3	9/1	--	--Labor Day--	--
	9/3	7	Superposition principle and expectation value	3
	9/5	8	Free particle and plane wave	4
4	9/8	9	1D particle in a box	4
	9/10	10	Review	--
	9/12	11	**Exam I**	--
5	9/15	12	2D and 3D particle in a box	4
	9/17	13	Quantum mechanics in real world	5
	9/19	14	Heisenberg's uncertainty principle	6
6	9/22	15	Harmonic oscillator	7
	9/24	16	2D rigid rotor, angular momentum	7
	9/26	17	3D rigid rotor, spherical harmonics	7
7	9/29	18	Vector model and space quantization	7
	10/1	19	General aspects of spectroscopy	8
	10/3	20	Vibrational spectroscopy	8
8	10/6	21	Review	--
	10/8	22	**Exam II**	--
	10/10	--	--Fall Break--	--
9	10/13	23	Rotational spectroscopy	8
	10/15	24	Hydrogen atom, solution of Schrödinger equation	9
	10/17	25	Hydrogen atom, quantum numbers	9
10	10/20	26	Hydrogen atom, atomic orbitals	9
	10/22	27	Many-electron atoms, orbital approximation	10
	10/24	28	Building-up principles and periodicity	10
11	10/27	29	Term symbols and atomic spectra	11
	10/29	30	Born-Oppenheimer approximation	12
	10/31	31	Hydrogen molecular ion, LCAO-MO	12
12	11/3	32	Homo- and hetero-nuclear diatoms	12
	11/5	33	Review	--
	11/7	34	**Exam III**	--
13	11/10	35	Hybrid orbitals	13
	11/12	36	Hückel approximation	13
	11/14	37	Electronic spectroscopy	14
14	11/17	38	Internal conversion and intersystem crossing	14
	11/19	39	Computational chemistry	15
	11/21	40	Symmetry elements	16
15	11/24	41	Symmetry groups	16
	11/26	42	Representation and character tables	16
	11/28	--	--Thanksgiving--	--
16	12/1	43	Applications of group theory	16
	12/3	44	Nuclear magnetic spectroscopy	17
	12/5	45	Review	--