Chemistry 76000: Introductory Quantum Chemistry
The Graduate Center of the City University of New York
Fall 2011

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Office Hours: Thursdays at the Graduate Center RM 4438 &
by appointment at Queens College (Office at QC: Science Building B312)

Lectures Tuesdays and Thursdays, 10:30 am -11:50 am, RM 8404 at the Graduate Center

Textbooks Ira N. Levine, *Quantum Chemistry*, 6th Ed., Prentice Hall, 2009 (required).
Supplementary materials will be provided in class and on line.

Other textbooks:
1. Donald A. McQuarrie and John D. Simon, *Physical Chemistry: A Molecular Approach*, University Science Books
(or Donald A. MaQuarrie, Quantum Chemistry, 2nd Ed, 2008)
2. John P. Lowe and Kirk Peterson, Quantum Chemistry, 3rd Ed, Elsevier

Course Description & Learning Goals

The goal of this course is to give doctoral graduate students in chemistry a solid understanding of the physical and mathematical aspects of quantum mechanics and molecular electronic structure. A basic familiarity with the concepts covered in undergraduate physical chemistry (e.g. *Physical Chemistry* by Peter Atkins and Julio De Paula, 8th Ed., Freeman), and a background in differential and integral calculus are required. Mathematical concepts including differential equations and linear algebra will be developed as needed in the course.

It is your responsibility to attend and to be punctual. I will not follow the Levine's textbook exactly. Homework assignments and exams and will be based on my lectures.

Detailed learning goals are subdivided into a number of topics as listed in the attached schedule, including understanding of the postulates of quantum mechanism, wavefunctions, operators and Schrödinger equation, the analytical solutions of time-independent Schrödinger equation for simple systems, the approximation methods for complex systems, etc.

Homework Weekly homework will be assigned every Tuesday (posted on line) and will be collected the following Tuesday. No credits will be given for late homework. You may work together on the homework assignments but the material handed in must be original and not copied from another individual. If duplicate assignments are received, no credits will be given.

Grading

Homework assignments	20 %
Three in-class exams	40 %
Final exam	40 %

Exam information

All exams are closed book/notes and no additional material may be consulted other than that provided with the examination sheet. No make-up exams will be given except in cases of documented legitimate reasons for absence. In the event of an excused absence from the final, contact the instructor and/or program office.

Exam I	Lectures covered:	Aug 30 - Sep 15
Exam II	Lectures covered:	Sep 22 - Oct 18
Exam III	Lectures covered:	Oct 27 - Nov 17

The final exam will be comprehensive and will draw from the entire semester's material.

Lecture Schedule and Topics

Date	Lecture Topics
Aug 30	Postulates and General principles of Quantum Mechanics: Wave Functions and Operators, and Mathematical Background
Sep 1	
Sep 6	
Sep 8	The Schrödinger Equation
Sep 13	Analytical Solutions: A Particle in a Box (One-dimensional)
Sep 15	Analytical Solutions: A Particle in a Box (Two-Dimensional/Three-Dimensional)
Sep 20	Exam I
Sep 22	Analytical Solutions: The Harmonic Oscillator and Vibrational Spectroscopy
Sep 27	
Oct 4	Follow a Friday Schedule
Oct 6	Analytical Solutions: The Rigid Rotator, Angular Momentum and Rotational Spectroscopy
Oct 11	
Oct 13	Analytical Solutions: Hydrogen Atom and Hydrogenlike Orbitals
Oct 18	
Oct 20	Exam II
Oct 25	Review of Mathematics: Determinants, Matrices, Linear Transformations and Matrix Eigenvalue Problem
Oct 27	Approximation Methods: Variation Method
Nov 1	
Nov 3	Approximation Methods: Perturbation Theory
Nov 8	
Nov 10	Helium Atom (I): Variation and Perturbation Treatments of the Ground State
Nov 15	
Nov 17	Helium Atom (II): Perturbation Treatment of the Excited States
Nov 22	Exam III
Nov 24	Thanksgiving recess
Nov 29	Electron Spin (I): The Spin-Statistics Theorem and the Pauli Exclusion Principle
Dec 1	Electron Spin (II): Slater Determinants
Dec 6	Many-Electron Atoms: Hartree-Fock SCF Method and Atomic Terms
Dec 8	Electronic Structure of Molecules
Dec 13	
Dec 19	Final Exam (9:30am-12:30 am)