Chem 486: Introductory Quantum Mechanics in Chemistry

Fall 2014

Lecture Hours: 11:00 AM - 12:15 PM Tuesday and Thursday (unless noted otherwise)
Lecture Room: VN G307

Office Hours: 1:00 PM - 2:00 PM Tuesday
Office Location: Caudill 018

Email: ykanai@unc.edu : Include “CHEM486” in Subject line.

Course Description

This course covers introductory quantum mechanics in context of chemistry, designed primarily for the first-year graduate students in chemistry and advanced undergraduate students. We will quantitatively discuss how various fundamental concepts in chemistry are derived from quantum theory. The course also lays a necessary foundation for comprehending topics covered in advanced/modern quantum chemistry, electronic structure theory, and molecular spectroscopy.

This subject can be truly comprehended only by actually working out its mathematics because of the non-intuitive nature of quantum mechanics. Lectures are used mostly to discuss fundamental equations and to derive important quantum-mechanical concepts from those equations in detail. Two or three problem sets will be given during the semester, and the students are required to turn them in on time. You will be given at least one week for each problem set. The instructor will discuss some questions from the problem sets in class when appropriate. The final exam will be largely based on the topics covered in the lectures and on the problem sets.

Mandatory Textbook
Quantum Chemistry by I. Levine.

Other Supplemental Textbooks
Molecular Quantum Mechanics by P. Atkins and R. Friedman
Introduction to Quantum Mechanics by D. Griffiths
Modern Quantum Mechanics by J. J. Sakurai
Topics

1. Review of Mathematics and Schrodinger Equation
2. Quantum Confinement and Tunneling
3. Quantum Mechanical Operators
4. Harmonic Oscillator and Ladder Operators
5. Angular Momentum and Atomic Orbitals
6. Theorems of Quantum Mechanics
7. Variational Principle
8. Perturbation Theory
9. Solids and Bloch Theorem
10. Other advanced topics

Grade

High Pass : > 95%
Pass : 95% ~ 81%
Low Pass : 80% ~ 70%
Fail : < 70%

For undergraduate students, the following grading scale will be used.

A: > 95%
A-: 95% ~ 91%
B+: 90% ~ 85%
B: 84% ~ 80%
B-: 79% ~ 75%
C+: 74% ~ 70%
C: 69% ~ 65%
C-: 64% ~ 60%
D+: 59% ~ 55%
D: 54% ~ 50%
F: < 50%

- The final grade may be curved favorably, based on the mean/average grade and class attendance.