Topics in Quantum Chemistry
CHEM 5500 (Fall 2022)

Times: M/W 8:00 to 9:25 am (starting 10/03)
Location: SLSRC 2410

Course Instructor: Dr. Ulrich H.E. Hansmann
Office: SLSRC 3410
Office hours: M/W after class or by appointment
Email: uhansmann@ou.edu
Course web site: http://hansmann-lab.com/cbpc/hansmann/5500.php

Description

The purpose of this course is to introduce fundamental concepts of quantum mechanics and its application in chemistry. The emphasis in the first half of the course (following the book by Levine) is on the postulates and theorems in quantum mechanics and contrasting classical vs. quantum behavior for simple systems. In the second half we look into modern quantum methods for solving molecular electronic structures. The course is directed toward graduate and advanced undergraduate students in physical chemistry, biochemistry, bioengineering and chemical engineering. The following concepts (among other) will be discussed:

1) Particle-wave duality, Schrödinger equation
2) Uncertainty principle and measurement outcomes
3) Operator formalism
4) Harmonic oscillator and other simple systems
5) Hydrogen atom
6) Variation method and perturbation theory
7) Fermions and bosons
8) Born-Oppenheimer approximation
9) Hartree-Fock theory

Pre-requisites

At least one undergraduate-level Physical Chemistry and one Calculus course are required, or consult with the lecturer.

Grading Scheme

Home work: 70% Final exam: 30%

Textbooks

- Ira N. Levine*, Quantum Chemistry*, Prentice Hall, Sixth Edition, 2008.

Make-up exam and home work extensions

Make-up exams or assignment deadline extensions will be given only under extreme circumstances and only with prior notification and documentation. There will be no extra credit assignments given.

University codes and policies of behavior

See "University policies regarding instruction" downloadable from the Provost's website,

http://www.ou.edu/provost/pronew/content/memorand.html

Each student should acquaint her or his self with the University's codes, policies, and procedures involving academic misconduct, grievances, sexual and ethnic harassment, and discrimination based on physical handicap.

Any student in this course who has a disability that may prevent him or her from fully demonstrating his or her abilities should contact me personally as soon as possible so we can discuss accommodations necessary to ensure full participation and facilitate your educational opportunities.

Academic Misconduct

Any form of academic misconduct, as specified in the Student Code at OU and in the Chemistry Department's Graduate Student Handbook, will be reported to the Department and the Dean for appropriate action.

Other notes

I reserve the right to change by addition and/or subtraction any and/or all materials contained in this syllabus. This includes, but is not limited to, course content, assignments, due dates, and portion(s) of the grade assigned to individual items within this course.