BGSU
Department of Chemistry
CHEM 614 Syllabus

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Lecture time: MWF 8:30 AM
Lecture room: Overman Hall 184
Office hours: Ksenija D. Glusac: MWF 9:30 AM (please try to use the scheduled office hours)
Pavel Kucheryavy: Th 6-8 PM

Course web page: http://personal.bgsu.edu/~kglusac

Textbooks: 1. *Quantum Chemistry* by Ira N. Levine, 5th edition, ISBN 0-13-685512-1;
2. *Elements of Quantum Mechanics* by Michael D. Fayer, ISBN 0-19-514195-4;

Learning Objective:

The objective of this course is to present the basic principles of quantum chemistry. Below is a complete list of course topics:

1. The Schrodinger equation (3 lectures) – historical background of quantum chemistry; uncertainty principle; time-dependent and time-independent Schrodinger equation.
2. The Particle in a Box (3 lectures) – intro to differential equations; particle in 1D box and in rectangular well; tunneling.
3. Operators (3 lectures) – intro to operators; eigenfunctions and eigenvalues; particle in a 3D box.
4. The Harmonic Oscillator (3 lectures) – 1D harmonic oscillator; vibrations of molecules.
5. Angular Momentum (3 lectures) – intro to vectors; angular momentum of a one-particle system.
6. The Hydrogen Atom (3 lectures) – two particle problem reduced to one-particle problem; rigid-rotor and molecular rotations; hydrogen atom; Zeeman effect.

7. Theorems of Quantum Mechanics (3 lectures) – Hermitian operators, Fourier expansion of wave functions; eigenfunctions of commuting operators; parity; superposition of states.
8. The Variation Method (3 lectures) – variation theorem; determinants; matrices.
9. Perturbation Theory (3 lectures) – nondegenerate and degenerate perturbation theory; helium atom; time-dependent perturbation theory; interaction of radiation and matter.
10. Electron Spin and Pauli Principle (3 lectures) – spin and H-atom; He-atom; Pauli exclusion principle; Slater determinants; perturbation and variation treatment of lithium ground state; spin magnetic moment.
11. Many-Electron Atoms (3 lectures) – Hartree-Fock method; electron correlation; the Condon-Slater rules.
12. Molecular Symmetry (3 lectures) – elements and operations of symmetry; point groups.
13. Electronic Structure of Diatomic Molecules (3 lectures) – Born-Openheimer approximation; hydrogen molecule ion; MO and VB theories.
14. The Virial Theorem and the Hellmann-Feynman Theorem (3 lectures) – the Virial Theorem and chemical bonding; the Hellman-Feynman theorem; electrostatic theorem.
15. Ab Initio and DFT Treatments of Molecules (3 lectures) - electronic terms of polyatomic molecules; basis functions; H_2O, methane, ethane, ethylene;
16. Semiempirical and Molecular-Mechanics Treatments of Molecules (3 lectures) – the Huckel method; the molecular mechanics methods.
17. Comparison of Methods (3 lectures) – geometry; energy; hydrogen bonding.

Grading: Three exams 45 % (each exam 15 %)
Final exam 20 %
Homework 15 %
Activity in classroom (20 %).
Grading Scale: A = above 90%, B = 80-90%, C = 68-79%, D = 51-67%, F = below 50%.

Dates: Homework is due two days after the chapter has been lectured.

Exam 1: Sep 18
Exam 2: Oct 16
Exam 3: Nov 13

Final: Dec 17, 8:30-10:30 am