Course: Chem 458/506 **Topic: Quantum Chemistry & Spectroscopy (Spring 2018)**

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ROOM: 213 Norton
TIME: Tue/Thu 11:00-12:20

CONTENTS*

Part I — Schedule

1. **Quantum Mechanics (QM) vs Classical mechanics. Postulates of QM. Application to chemical atomic systems: Schrodinger equation for hydrogen atom and its solution. Quantum numbers. Selection rules. Spin. Uncertainty principle.** — **January 30, Feb 1 (Prasad)**

2. **Many electron atoms and electron-electron interaction; Pauli's principle. Hartree-Fock method for many electron systems. Electronic configuration of many-electron atoms. Popular Quantum Chemistry codes. Semi-empirical methods.** — **February 6, 8 (Prasad)**

3. **Approximate methods for complex chemical systems. Variation and perturbation treatments; examples of each calculations of first and second order perturbation terms.** — **February 13, 15(Baev)**

4. **Molecular systems: partitioning of molecular Hamiltonian into electronic, vibrational and rotational terms by using Born-Oppenheimer approximation.** — **February 20, 22 (Baev)**

5. **Valence Bond (V.B) vs. Molecular orbitals (MO): Homo-nuclear and heteronuclear diatomic molecules. More sophisticated molecules and symmetry requirements.** — **February 27, March 1 (Prasad, Baev)**

EXAM I — **March 6**

Part II

1. **A brief introduction to symmetry and group theory: symmetry elements; point groups representations; character tables. Applications of group theory.** — **March 8, 13 (Baev)**

2. **Brief discussions of following topics:** **March 15, March 27 (Prasad, Baev)**
   Ligand field theory.
   Electronics structure of electron-deficient molecules
   π-electron theory of organic molecules, Huckel's treatment
   More sophisticated MO treatments

3. **Density Functional Theory for atomic and Molecular Clusters.** **March 29, April 3 (Baev)**

4. **Nanomaterials; Quantum Dots, Metallic Nanoparticles and Plasmonics** **April 5, April 10 (Prasad)**

Part III

1. **Spectroscopy: confirmation of quantum mechanical predictions;** **April 12, 19 (Prasad, Baev)**
   energy states and transitions; interaction between molecules and radiation, dipole allowed transitions;
   Raman transitions; population inversion and lasers.

EXAM II **April 17**

2. **Multi-photon processes.** **April 24 (Prasad)**
   Nonlinear optical effects and applications

3. **Electronic spectroscopy and structure** **April 26, May 1 (Prasad, Baev)**

4. **Vibrational spectroscopy, IR and Raman** **May 3, 8, 10 (Baev)**

EXAM III **May 15**

- Each Exam is 1 hour and 20 minutes and only covers the new materials. Each Exam is also equally weighted (100 points each)

Text Book

1. **"*Quantum Chemistry and Spectroscopy*" T. Engel, Prentice Hall (2010)**

   Supplementary Book:
   "Quantum Chemistry" I.N. Levine, Fifth Edition, Prentice Hall (2000)