Course: Chem 506 (Spring 2017) **Topic: Quantum Chemistry & Spectroscopy**

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ROOM: 508 Cooke
TIME: Tuesday, Thursday, 11:00AM-12:20PM

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 31, Feb 2 (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 7, 9 (Prasad)**
3. Approximate methods for complex chemical systems. Variation and perturbation treatments; examples of each calculations of first and second order perturbation terms.	**February 14, 16 (Baev)**
4. Molecular systems: partitioning of molecular Hamiltonian into electronic, vibrational and rotational terms by using Born-Oppenheimer approximation.	**February 21, 23 (Baev)**
5. Valence Bond (V.B) vs. Molecular orbitals (MO): Homo-nuclear and heteronuclear diatomic molecules. More sophisticated molecules and symmetry requirements.	**February 28, March 2 (Baev)**
EXAM I	**March 7**
Part II	
1. A brief introduction to symmetry and group theory: symmetry elements; point groups representations; character tables. Applications of group theory.	**March 9, 14 (Baev)**

2. **Brief discussions of following topics:** **March 16, March 28 (Prasad)**
   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 30, April 4 (Baev)**

4. **Nanomaterials; Quantum Dots, Metallic Nanoparticles and Plasmonics** **April 6, April 11 (Baev)**

EXAM II **April 13**

Part III

1. **Spectroscopy: confirmation of quantum mechanical predictions;** **April 18, 20 (Prasad)**
   energy states and transitions; interaction between molecules and radiation,
   dipole allowed transitions;
   Raman transitions; population inversion and lasers.

2. **Multi-photon processes.** **April 25 (Prasad)**
   Nonlinear optical effects and applications

3. **Electronic spectroscopy and structure** **April 27, May 2 (Prasad, Baev)**

4. **Vibrational spectroscopy, IR and Raman** **May 4, (Prasad) May 9,(Baev)**

   May 11, (Prasad)

EXAM III **May 16**

- 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)