**BIRLA INSTITUTE OF TECHNOLOGY AND SCIENCE, PILANI**
**INSTRUCTION DIVISION**
**First SEMESTER 2015-2016**
**Course Handout (Part II)**

Date: 25.07.2015

In addition to part I (General Handout for all courses appended to the time table) this portion gives further specific details regarding this course.

**Course No.** : **CHEM F 213**
**Course Title** : **Physical Chemistry - II**
**Instructor-in-charge** : **Shamik Chakraborty**

**Objective of the course:** The course provides an introduction to quantum mechanics and application of quantum mechanics to electronic structure of atoms, chemical bonding, molecules, and spectroscopy.

**Text Book (TB):** Quantum Chemistry, Donald A McQuarrie, University Science Books (First Indian Edition 2003, Viva Books Private Limited)

**Reference Books (RB): RB-1**: Quantum Chemistry, Ira N. Levine, 7$^{th}$ Edition, PHI, 2014, **RB-2**: Quantum Mechanics, Bransden and Joachain, 2$^{nd}$ Edition, Pearson. **RB-3:** Atkins' Physical Chemistry, 9$^{th}$ Edition, Peter Atkins and Julio De Paula, Oxford University Press.

**Course Plan:**

- **Development of Quantum Theory: L-01 to L-05**
  - **Lecture – 01 (L-01): Failure of classical theory and origin of quantum theory**
    - Learning objectives: Blackbody radiation, Photoelectric Effect, Atomic Vibrations in Crystals, Line Spectra and Bohr Model of H Atom, de Broglie's postulate, Heisenberg uncertainty principle.
    - Learning outcome: Recognize the need for quantum theory.
    - Reference: TB, 1.1 – 1.4
    - Date(s):
  - **Lecture – 02 (L-02): The wave equation**
    - Learning objectives: Motion of vibrating string, separation of variables, normal modes, superposition, Fourier series.
    - Learning outcome: Know mathematical background for quantum theory.
    - Reference: TB, 2.1 – 2.5
    - Date(s):

- **Lecture – 03 (L-03) to Lecture – 05 (L-05): Postulates of quantum mechanics**
    - Learning objectives: Wave function, Schröndinger equation, operators and observables, eigenvalue problem, time evaluation and stationary states, uncertainty, measurement and superposition of states.
    - Learning outcome: Consolidate new concepts to be used in quantum mechanics.
    - Reference: TB, 3.1 – 3.4, 3.7, 3.8, 3.11, 4.1 – 4.9; RB-2, 7.1 – 7.10.
    - Date(s):

- **Some exactly solvable problems: L-06 to L-17**
  - **Lecture – 06 (L-06) to Lecture – 07 (L-07): Particle in a box (PIB)**
    - Learning objectives: Bound states, Zero point energy, symmetry, superposition states, and degeneracy in two- and three- dimensions.
    - Learning outcome: Theorize quantization of states and zero point energy in very simple systems, like, PIB.
    - Reference: TB, 3.4 – 3.11, 6.1 – 6.2
    - Date(s):
  - **Lecture – 08 (L-08) to Lecture – 09 (L-09): Finite potential wells and barriers**
    - Learning objectives: Bound states in wells, probability current, reflections and tunneling.
    - Learning outcome: Recognize working principle of scanning tunneling microscopy.
    - Reference: Study materials; RB-2, 2.5; RB-3, 8.3.
    - Date(s):
  - **Lecture – 10 (L-10) to Lecture – 12 (L-12): Harmonic oscillator**
    - Learning objectives: Eigen states for simple harmonic oscillator, zero point energy, molecular vibration, dissociation energy, anharmonicity.
    - Learning outcome: Define vibrational spectroscopy of molecules.
    - Reference: TB, 5.1 – 5.13.
    - Date(s):
  - **Lecture – 13 (L-13) to Lecture – 15 (L-15): Angular momentum and rigid rotor**
    - Learning objectives: Energy levels, operator for angular momentum, commutation relation, wavefunction, and molecular rotation.
    - Learning outcome: Define rigid rotator as model for rotating diatomic molecules.
    - Reference: TB, 6.3 – 6.7, 6.10
    - Date(s):
  - **Lecture – 16 (L-16) to Lecture – 17 (L-17): The hydrogen atom**
    - Learning objectives: Energy levels, wavefunction – angular and radial parts, orbitals, and effect of magnetic field on hydrogen atom.
    - Learning outcome: Review atomic orbital picture of H-atom from quantum mechanics.
    - Reference: 6.8 – 6.11
    - Date(s):

- **Approximation methods: L-18 to L-22**
    - **Lecture – 18 (L-18) to Lecture – 20 (L-20): Variation method**
        - Learning objectives: Schrödinger equation for He-atom cannot be solved exactly, variation theorem, linear variation method.
        - Learning outcome: Evaluate the upper bound to the ground state energy of a system.
        - Reference: 6.12, 7.3 – 7.7, 8.1, 8.2
        - Date(s):
    - **Lecture – 21 (L-21) to Lecture – 22 (L-22): Perturbation theory for stationary state**
        - Learning objectives: Systematic correction of wavefunction and energies of non-degenerate states.
        - Learning outcome: Calculate ground state energy of various systems from the unperturbed state of the system.
        - Reference: TB, 7,1, 7.2, 8.2; RB-2, 9.1 – 9.7
        - Date(s):
- **Many electron atoms: L-23 to L-28**
    - **Lecture – 23 (L-23): Many electron wavefunction**
        - Learning objectives: Systems of identical particles, spin and permutation symmetry, Pauli principle, and Slater determinants.
        - Learning outcome: Define spin as another coordinate.
        - Reference: TB, 8.4 – 8.6
        - Date(s):
    - **Lecture – 24 (L-24) to Lecture – 26 (L-26): SCF method**
        - Learning objectives: Hartree and Hartree-Fock methods, electronic structure calculations, comparison with experimental data, periodicity.
        - Learning outcome: Recognize theoretical concepts behind electronic structure calculations of polyatomic molecules.
        - Reference: TB, 8.3, 8.7, 8.8
        - Date(s):
    - **Lecture – 27 (L-27) to Lecture – 28 (L-28): Atomic terms and spectra**
        - Learning objectives: Addition of angular momenta, spin-orbit interaction, absorption and emission spectra of atoms, selection rules.
        - Learning outcome: Examine allowed and forbidden transition in atoms.
        - Reference: TB, 8.9 – 8.12
        - Date(s):
- **Molecules: L-29 to L-36**
    - **Lecture – 29 (L-29): Born-Oppenheimer approximation**
        - Learning objectives: Separation of nuclear and electronic motion.
        - Learning outcome: Express molecular wavefunction as product of nuclear and electronic wavefunctions.
        - Reference: TB, 9.1
        - Date(s):

- **Lecture – 30 (L-30) to Lecture – 31 (L-31): Valence Bond Theory – $H_2$**
  - Learning objectives: Localized electron pair bonds.
  - Learning outcome: Demonstrate successful description of chemical bond.
  - Reference: TB, 9.2 – 9.5
  - Date(s):
- **Lecture – 32(L-32) to Lecture – 33 (L-33): Molecular Orbital Theory – $H_2^+$, $H_2$**
  - Learning objectives: Linear combination of atomic orbitals, comparison to valence bond picture.
  - Learning outcome: Illustrate application of molecular orbital theory to diatomic molecules.
  - Reference: 9.6 – 9.8
  - Date(s):
- **Lecture – 34(L-34) to Lecture – 36 (L-36): Homonuclear diatomic molecules**
  - Learning objectives: Molecular electronic configuration, Pauli principle, SCF-LCAOMO wavefuncitons, and molecular terms.
  - Learning outcome: Compare experimental observations along with theoretical prediction for diatomic molecules.
  - Reference: TB, 9.9 – 1.5
  - Date(s):
- **Lecture – 37(L-37) to Lecture – 38 (L-38): Hückel MO theory**
  - Learning objectives: π-electron approximation for conjugated systems, energies and delocalization, atomic charge distribution and bond order.
  - Learning outcome: Explore quantum chemical approximation of aromatic systems.
  - Reference: TB, 9.21 – 9.24.
  - Date(s):

- **Molecular spectroscopy: L-39 to L-42**
  - **Lecture – 39(L-39): Electromagnetic radiation and its interaction with molecules**
    - Learning objectives: Perturbation theory of degenerate energy levels, time dependent perturbation theory, interaction of radiation and matter, absorption, emission.
    - Learning outcome: Recognize quantum-mechanical approach for spectroscopy.
    - Reference: RB-2, 9.5, 9.9, 9.10
    - Date(s):
  - **Lecture – 40(L-40): Rotational and vibrational spectra**
    - Learning objectives: Different regions of electromagnetic spectrum, molecular rotation, molecular vibration, normal modes, rotational transitions accompany vibrational transitions, Boltzman population distribution.
    - Learning outcome: Explain rotational and vibrational spectroscopy.

    - Reference: TB, 10.1 – 10.10; study materials
    - Date(s):
- **Lecture – 41(L-41): Electronic spectra**
    - Learning objectives: Electronic states, transitions, vibrational and rotational information, intensity pattern.
    - Learning outcome: Recognize fundamentals of electronic spectroscopy.
    - Reference: TB, 10.11 – 10.13, Study materials.
    - Date(s):
- **Lecture – 42(L-42): Selection rules and Franck-Condon principle**
    - Learning objectives: Overlap integrals, nuclear motion can be factored approximately into a rotational part and vibrational part, selection rule in rigid rotor, selection rule in harmonic oscillator, selection rule in electronic spectroscopy.
    - Learning outcome: Formulate allowed and forbidden transition.
    - Reference: 10.14 – 10.18
    - Date(s):

**Learning outcome of the course:**

1. Demonstrate the need of quantum mechanics to explain atomic and molecular phenomenon.
2. Explain bonding theories and their application to simple molecular systems.
3. Illustrate various approximation methods using quantum mechanics.
4. Formulate SCF methods for many electron system which is the basic of any electronic structure calculation for geometry optimization and energy calculation.
5. Application of quantum mechanics into molecular spectroscopy.

**Tutorials:** The tutorial hour will be utilized for overall review of the topics covered in the lectures, and problem solving. Some of the problems discussed/solved in the tutorial may be included in the evaluation. In addition, a part of the continuous evaluation will also be conducted during tutorial hour.

**Problem sets**: There will be several problem sets in this course. One of the efficient ways to learn quantum mechanics is to derive expression and solve problems on your own. After you have spent significant time working on all of the problems independently, you may confer with your classmates or with Dr. Chakraborty. However, you need to write up the solutions to the problems on your own.

**In-class problem**: There will be several in-class problems as well. Volunteers will be asked to solve those problems on the board. This is not meant for any situation to put you under pressure, rather is meant to provide you an interactive environment for problem solving. Participation of all students is expected.

**Electronic structure calculation program**: Hands-on-training to electronic structure calculation programs will be provided as part of the course. These sessions will be conducted beyond regular class and tutorial hours and will not be evaluative.

**Attendance policy**: It is expected that students will attend all scheduled lectures. Students are responsible for the topics covered in the lectures as well as worksheets, assignment, and take home problem sets distributed during lecture.

**Evaluation Scheme:**

| Component | Duration | Weightage (%) | Date & Time |
|---|---|---|---|
| Mid Semester Test | 90 minutes | 25 | 5/10 8:00 - 9:30 AM |
| Assignment/Quiz | | 35 | Continuous |
| Comprehensive Examination | 180 minutes | 40 | 1/12 FN |

**Consultation Hour:** T Th 11.00 hrs. - 12.00 hrs., by appointment or just stop by

**e-mail of the instructor**: shamik@pilani.bits-pilani.ac.in

**Notice:** Notices concerning this course will be displayed on the Department of Chemistry Notice Board.

**Make-up Policy:** Refer to Part-I of the handout for details.

**Instructor-in-charge,**
**CHEM F412**