Chemistry 218 **Spring 2015-2016**
Molecular Structure *R. Sultan*

COURSE SYLLABUS

- **Email:** *rsultan@aub.edu.lb*
  Homepage: *http://staff.aub.edu.lb/~rsultan/*

- **Lectures:** 12:30-13:45 T, Th. 101 Chemistry

- **Textbook:** P. W. Atkins and J. de Paula, Physical Chemistry, 10th edition, Oxford University Press (2014), + Solutions Manual (Atkins, Ch. Trapp, M. Cady and C. Giunta).
  Chem. 218 covers Part 2 (**STRUCTURE**, Chapters 7-10, 12, 13).

- **Office Hours:** *Monday* (12:30-1:30) - *Wednesday* (1-2) - *Thursday* (2:30-3:30). – **Room 518 Chemistry**

- **Reference Books:**

  1. I. N. Levine, Quantum Chemistry, Prentice Hall (NJ 2008), 6th edition.
  2. D. A. McQuarrie and J. D. Simon, Physical Chemistry: a Molecular Approach, University Science Books, (CA 1997).

- **Problems:** Problem sets will be distributed throughout the semester (from Atkins + auxiliary problems).
  Problem Sets and their *Solutions* They will also be accessible on **MOODLE.** You must solve all the assigned problems in a gradual manner, i.e. parallel to the advancement in the course material.

- **Grading**:

  2 Quizzes: 50% (Best: 30%, Lower: 20%)
  Computational Project 15% (Prof. Faraj Hasanayn)
  Final Exam: 35%

- **Quiz Dates:**

  Quiz I Tuesday March 8, 2016
  Quiz II Tuesday April 12, 2016
  Project Thursday April 14, 2016
  Final To be announced later

- Last day of withdrawal: Thursday March 31, 2016
- Last day of classes: Monday May 2, 2016
- Last day of finals: Saturday May 14, 2016

- **LEARNING OUTCOMES**: The students should achieve the following:

1. Become familiar with the physical phenomena discovered near the beginning of the 20th century, which led to the development of Quantum theory.
2. Master the basic concepts in Quantum Mechanics in a durable manner. You should be able to formulate a quantum mechanical problem by writing the Schrödinger equation for the specific chemical system under study, and understand the possible routes for its solution.
3. Master the technique of operator analysis, and understand the mathematical formalism of Quantum theory, with a preliminary exposure to matrix formulation.
4. Understand the basic models suitable for the possible simulation of chemical problems in energetics and bonding, such as the free particle and the particle in-a-box (translation), the harmonic oscillator (vibration), and the particle on-a-ring (rotation).
5. Assimilate advanced quantum mechanical concepts that emerge from the treatment of simple chemical systems (atoms and molecules), such as **atomic orbitals, atomic states, electronic configuration, term symbols, atomic spectra** (atoms), and their analogs for molecules.
6. Learn the quantum mechanical formulation of simple molecules and subsequently the basis for ***chemical bonding*** and the emerging concepts, such as **molecular orbitals, hybridization, molecular states, term symbols, conjugation, aromaticity, molecular spectra** (molecules).
7. Understand the basics and fundamentals of rotation, vibration and electronic spectroscopy.
8. **Acquire, develop and master a problem solving strategy in all the covered material** (see paragraphs on **Problems** and **Solutions** in the previous section).

COURSE CONTENTS

SUBJECT	SECTION IN ATKINS
QUANTUM THEORY	
Central ideas in classical mechanics	Foundations - B1.a-c
Failures of classical mechanics – Idea of energy quantization	7A.1
Blackbody radiation - Heat capacities of	7A.1

solids - Atomic and molecular spectra	
Wave-particle duality Photoelectric effect - Electron diffraction - DeBroglie's relation Schrödinger wave equation (SWE)	7A.1
Born interpretation	7B
Postulates of Quantum Mechanics	7C
Operators and observables	7C.1
Superposition and expectation values	7C.2
Uncertainty principle	7C.3
Translational motion	**8A**
Free particle - Particle in-a-box	8A.1-3
Tunneling	8A.4
Vibrational motion	**8B**
Simple harmonic oscillator (SHO)	8B.1
Rotational motion	**8C**
Particle on-a-ring -	8C.1
Space quantization of angular momentum	8C.2
Rotation in three dimensions - The vector model Spin	8C.2.e
ATOMIC THEORY	
Structure and Spectra of Hydrogenic atoms	9A
Quantum mechanical interpretation	9A.1
Atomic orbitals Shells and subshells	9A.2
Quantum mechanical calculations (H-atom) Spectral transitions - Selection rules	9A.2
Helium atom - Orbital approximation SPIN- Pauli exclusion principle	9B.1
Penetration and shielding	9B.1.c
Many-electron atoms – Aufbau principle	9B.2
SCF orbitals (*Reading*)	9B.3
Atomic Spectra	**9C**

Spectra of complex atoms	9C.1
Singlet and triplet states	9C.2.a
Spin-orbit coupling - Fine structure	9C.2.b
Atomic term symbols	9C.2.c
Spectral selection rules	9C.2.e
Effect of magnetic field - Zeeman effect	Problem 9C.9
MOLECULAR STRUCTURE	
Valence bond (VB) theory (*Reading*)	10A
Molecular Orbital (MO) Theory	
H_2^+ molecule-ion	10B
MO-LCAO treatment- Variation principle	10B
VB Theory – H_2 molecule	10A
Homonuclear diatomic molecules Classification of molecular orbitals (σ- and π- orbitals)	10C
Heteronuclear diatomics	10D
Polyatomic molecules	Outside references
Molecular term symbols	**13A.1**
Hybridization	10A.2.B
Hückel MO π-electron theory	**10E.1**
Conjugation – Armoaticity	10E.2
Computational Chemistry (*Reading*)	10E.3
SPECTROSCOPY	
Experimental techniques (*Reading*)	12A
Features of spectroscopy (*Reading*)	12A
ROTATION SPECTRA	**12B & C**
Moments of inertia	12B.1
Rotational energy levels	12B.2
Spherical top molecules	12B.2.a
Symmetric tops - Linear molecules - Degeneracy	12B.2.b 12B.2.c
Centrifugal distortion	12B.2.d
Rotational transitions - selection rules	12C.1.a
Appearance of rotational spectra	12C.1.b

VIBRATION SPECTRA	**12D**
Harmonic oscillator - vibrational energy levels	12D.1
Selection rules	12D.2
Morse potential - Anharmonicity	12D.3
Ro-vibrational spectra of diatomic molecules	12D.4
ELECTRONIC SPECTRA	**13A**
Diatomic molecules	13A.1
Term Symbols - Electronic excited states of molecules	13A.1.a
Spectral transitions & selection rules	13A.1.b
Vibrational structure - Franck-Condon principle	13A.1.c
Rotational structure	
Fates of electronically excited states - Fluorescence and Phosphorescence	13B