

## NOTES TO STUDENTS

Dear Students,

I hope and pray that you all are safe at home.

During this semester, I have taught the following topics:

1. Recapitulation of postulates and Theorems of Quantum Mechanics
2. Particle-in-a-box problem including Free Electron Model, 2-D and 3-D boxes
3. Quantum Mechanical Tunneling
4. Particle-on-a-ring
5. Harmonic Oscillator- Operator method including proof of virial theorem, average values.
6. Some applications of time-independent perturbation theory
7. Variation theorem applied to various systems
8. Hydrogen atom and calculation of various properties from the radial part.
9. Angular momentum and spherical harmonics
10. Helium atom: Ground and Excited states
11. Photoelectron spectroscopy of atoms and Koopmans' theorem
12. Bonding: solution for  $H_2^+$ : hydrogen molecule by valence bond and molecular orbital theory, Configuration interaction
13. MO theory applied to second row homonuclear diatomics and heteronuclear diatomics. Photoelectron spectroscopy of molecules
14. Bonding in second row dihydrides. Walsh Diagrams
15. HMO Theory: Incomplete

I have already submitted the assignment for the covered topics for uploading at the website.

Before the mid-Semester break, I had started HMO theory and discussed HMO treatment of simple molecules like ethylene, allyl system, butadiene and cyclopropenyl covering about two lectures.

I am now uploading reading material for the next few topics in HMO theory. Lecture 3 of HMO theory is about simple acyclic systems. Some concepts are discussed and applied to the allyl system and butadiene and their ion radicals.

In Lecture 4, longer acyclic systems are discussed, as well as cyclic systems and their generalizations. You will need some background on linear independence of vectors and Gram-Schmidt orthogonalization. If this topic was not taught to you in Paper 103 of First Semester, please refer to my class-notes from students of my class.

The next few lectures will give advanced applications, including extension to heteroatom systems.

Each lecture is of one hour duration. Some questions are asked during and after the write-up. These will cover another hour of your time. Please solve these and get back to me in case of any difficulty. These will help you understand the topics better. All the material you need is there in the write-up.

Keep on watching the website for more study material. After HMO theory, the last topic to be covered is Introduction to Computational Chemistry.

For my lectures on Elementary Quantum Mechanics, you may go to the site

<https://www.youtube.com/watch?v=Vja5RFSqCM4>

<https://www.youtube.com/watch?v=-6-i-nP59f0>

<https://www.youtube.com/watch?v=CSang2re37c>