Atomic Structure and Chemical Bonding

SWAYAM Prabha Course Code NPTEL-S7

PROFESSOR'S NAME	Prof. K. Mangala Sunder
DEPARTMENT	Chemistry
INSTITUTE	IIT Madras
COURSE OUTLINE	The course is a rigorous introduction to principles of quantum chemistry and also describes all mathematical details at the introductory level, accurately however. It is limited to elementary model problems, angular momentum and spin and an introduction to chemical bonding in one and two-electron systems.

COURSE DETAILS

S. No	Module ID/ Lecture ID	Lecture Title/Topic
1	Lecture 1	Introduction
2	Lecture 2	Elementary Mathematical Functions Used in Our Course
3	Lecture 3	Schrodinger Equation: Particle in a One Dimensional Box
4	Lecture 4	Particle in a One dimensional Box: Probabilities and Expectation Values
5	Lecture 5	Elementary Mathematics: Introduction to Matrix Algebra - Part 1
6	Lecture 6	Elementary Mathematics: Introduction to Matrix Algebra - Part 2
7	Lecture 7	Elementary Mathematics: Matrix Eigenvalues and Eigenfunctions: Part I
8	Lecture 8	Elementary Mathematics: Matrix Eigenvalues and Eigenfunctions: Part II
9	Lecture 9	Particle in a Two Dimensional Box (Infinite Barrier)
10	Lecture 10	Heisenberg's Uncertainty Principle

11	Lecture 11	Expectation Values and Postulates in Quantum Mechanics
12	Lecture 12	Problems and Solutions for Particle in One and Two Dimensional Boxes
13	Lecture 13	Linear Vector Spaces: Matrix Representations
14	Lecture 14	Linear Vector Spaces and Operators: Diracâ€™s Bracket Notation
15	Lecture 15	Simple Harmonic Oscillator: Classical Hamiltonian
16	Lecture 16	Simple Harmonic Oscillator: Quantum Mechanical Solutions
17	Lecture 17	Simple Harmonic Oscillator: Wave Functions, Probabilities and Average Values
18	Lecture 18	Simple Harmonic Oscillator: Average Values for Position and Momentum
19	Lecture 19	Particle on a Ring: The Quantum Model
20	Lecture 20	Particle on a Ring: Expectation Values for Angular Momentum
21	Lecture 21	Coordinate Transformation
22	Lecture 22	Problems and Solutions for Harmonic Oscillator
23	Lecture 23	Hydrogen Atom: The Hamiltonian in Spherical Polar Coordinates
24	Lecture 24	Hydrogen Atom: Separation of the SchrÃ¶dinger Equation
25	Lecture 25	Hydrogen Atom: Radial and Angular Solutions and Animations Part I
26	Lecture 26	Hydrogen Atom: Radial and Angular Solutions and Animations Part II
27	Lecture 27	Hydrogen Atom: Radial Solutions and Probabilities
28	Lecture 28	Power Series Method for Differential Equation - I
29	Lecture 29	Hermiteâ€™s Differential Equation
30	Lecture 30	Legendre and Associated Legendre Equation

31	Lecture 31	Born-Oppenheimer Approximation
32	Lecture 32	Introduction to Angular Momentum
33	Lecture 33	Spin Â½ Angular Momentum
34	Lecture 34	Spin Angular Momentum and Coupling of Two Spin-1/2 Angular Momenta
35	Lecture 35	Coupling of Two Angular Momenta
36	Lecture 36	Video Tutorial for Hermite polynomials and hydrogen atom Part 1
37	Lecture 37	Video Tutorials Part 2
38	Lecture 38	Variational Principle in Quantum Chemistry: Linear superposition Principle
39	Lecture 39	Introduction to Variational Principle in Quantum Chemistry
40	Lecture 40	Variational Method: Method of Lagrange Multipliers
41	Lecture 41	Hydrogen Molecule Ion: The Molecular Orbital Method
42	Lecture 42	Hydrogen Molecule Ion: Calculations and Results
43	Lecture 43	Hydrogen Molecule: The Valence Bond Method
44	Lecture 44	Hydrogen Molecule: Calculations and Molecular Orbital Method
45	Lecture 45	Video Tutorials on Angular Momentum (Orbital and Spin) and Variational Method Part 1
46	Lecture 46	Video Tutorials on Angular Momentum (Orbital and Spin) and Variational Method Part 2
47	Lecture 47	Introduction to Quantum Mechanical Perturbation Theory
48	Lecture 48	First Order Time Independent perturbation Theory for Non-Degenerate states

49	Lecture 49	First and Second Order Time Independent Perturbation Theory for Non-Degenerate States
50	Lecture 50	First and Second Order Time Independent Perturbation Theory: Simple Examples
51	Lecture 51	Time Independent Perturbation Theory for Degenerate States: First Order
52	Lecture 52	General MO method for Homonuclear Diatomic Molecules
53	Lecture 53	General MO method for Heteronuclear Diatomic Molecules
54	Lecture 54	Introduction to Hybridization and Valence Bond for Polyatomic Molecules
55	Lecture 55	Huckel Molecular Orbital Theory I

References if Any:

1. Quantum Chemistry by Donald A. McQuarrie, Viva Books, 2011, Indian Edition.

2. Quantum Chemistry by R. K. Prasad, New Age Publications, 2011.

3. Mathematics for Physical Chemistry by D. A. McQuarrie, University Science Books, 2008

Instructor Contact Details:

Dr. K. Mangala Sunder, Ph. D. (McGill)

Professor and Head, Department of Chemistry and

Chief Coordinator, DTH SWAYAM Prabha, Ministry of Human Resource Development (2016-)

National Web Courses Coordinator, NPTEL, Ministry of HRD (2003 - 2015)

Indian Institute of Technology Madras, Chennai 600036

Email: mangal@iitm.ac.in; 044-22574220; mangalasunderk@gmail.com