



CHEMISTRY: ATOMIC STRUCTURE AND CHEMICAL BONDING

PROF. K. MANGALA SUNDER
Department of Chemistry
IIT Madras

TYPE OF COURSE : Rerun | Core | UG
COURSE DURATION : 12 weeks (24 Jan' 22 - 15 Apr' 22)
EXAM DATE : 23 Apr 2022

PRE-REQUISITES : Mathematics –integral and differential calculus (minimally, one variable), elementary first order differential equations and Matrix algebra—Eigenvalue –eigen vector analysis; Introduction to modern physics –Planck's radiation law, Einstein's theory on photoelectric effect and wave particle duality.

INTENDED AUDIENCE : B. Sc. Third Year / M. Sc. I Year

INDUSTRIES APPLICABLE TO : This is a core course. I do not expect any industry to be a specific sponsor

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.

ABOUT INSTRUCTOR :

Prof. K. Mangala Sunder joined IIT Madras as Assistant Professor in 1996 and became a Professor of Chemistry in IIT Madras since 2006. He is a native of Tirunelveli District, Tamil Nadu and had his early education in that district.

He was a trainee of the 23rd batch (1979) of Training Schools conducted annually by the Bhabha Atomic Research Centre before serving the Centre as a Scientific Officer for 2 years.

He obtained his PH. D. degree from McGill University in spherical tensor theory of solid state nmr spectroscopy under the mentorship of Prof. Bryan C. Sanctuary in the Chemistry Department.

He did his postdoctoral research in the University of British Columbia, Vancouver, Université de Montréal, Montréal and Queen's University, Kingston, Canada before returning to India in 1996.

COURSE PLAN :

Week 1 : Historical introduction to Quantum chemistry; a brief description of Planck's radiation law, study of photoelectric effect by Einstein, Hydrogen atom model by Niels Bohr and formal introduction to matter waves through de Broglie's proposal

Week 2 : The time dependent and time independent Schrödinger wave equation. Simple illustrations using matter waves.

Week 3 : The particle in a one dimensional and multi-dimensional potential-free box. Solutions and interpretations. Definitions of expectation values and probabilities.

Week 4 : Particle on a ring and angular momentum in quantum mechanics. Introduction to the abstract concept of spins and abstract states in quantum mechanics.

Week 5 : The harmonic oscillator, eigenvalues and eigenfunctions.

Week 6 : Introduction to vectors through matrices. Linear vector spaces and matrix methods for vectors. Special matrices, eigenvalues and eigenvectors of matrix and the relation to quantum mechanics.

Week 7 : The hydrogen atom. Formulation of the problem and separation of the Schrödinger equation using spherical polar coordinates.

Week 8 : The hydrogen atom. Solutions of the Schrödinger equation and their visualizations. Expectation value calculations.

Week 9 : Elementary Introduction to angular momentum in quantum mechanics and the spin states of two coupled spin-1/2 systems (two-electron spin states).

Week 10 : Born-Oppenheimer approximation and introduction to bonding concepts. The hydrogen molecule ion and simple analysis of molecular states.

Week 11 : The hydrogen molecule and the concept of linear combination of atomic orbitals.

Week 12 : Review and Summary.