QUANTUM CHEMISTRY OF ATOMS AND MOLECULES

PROF. ANINDYA DATTA
Department of Chemistry
IIT Bombay

TYPE OF COURSE : New | Elective | UG
COURSE DURATION : 12 weeks (20 Jul' 20 - 9 Oct' 20)
EXAM DATE : 17 Oct 2020

INTENDED AUDIENCE : Chemistry, Physics, 1st year Engineering

COURSE OUTLINE :
The course introduces students to quantum Chemistry. The syllabus is as follows.
Black body radiation. Failure of classical mechanics. Marsden experiment and Rutherford theory. Hydrogen atom spectrum. Bohr Sommerfeld theory. Uncertainty principle. Wave particle duality. Schrodinger equation. Postulates of quantum mechanics. Born approximation. Origin of quantization: Particle in a box, particle in a ring. Hydrogen atom. Atomic orbitals. Many electron atoms. Introduction to spin. Slater determinants. Self consistent fields. Valence bond and molecular orbital theories. Molecular orbitals of homonuclear and heteronuclear diatomic molecules. VSEPR. Molecular orbital and Valence bond approaches to polyatomic molecules. Hybrid orbitals. Huckel theory. Introduction to approximation methods. Scope of further study.

ABOUT INSTRUCTOR :
Prof. Anindya Datta is a Professor of Chemistry in IIT Bombay, with research interest in ultrafast spectroscopy and time resolved fluorescence microscopy. He has a teaching experience of 17 years. 15 Ph. D. students have been graduated from our laboratory. Eight more are working towards their degree. He received Excellence in Teaching Award from our institute in 2017 and also taught three NPTEL courses on Molecular Spectroscopy, Symmetry in Chemistry and Laser spectroscopy.

COURSE PLAN :

Week 1**:** Black body radiation. Failure of classical mechanics. Marsden experiment and Rutherford theory.

Week 2**:** Hydrogen atom spectrum. Bohr Sommerfeld theory. Uncertainty principle. Wave particle duality.

Week 3**:** Schrodinger equation. Born approximation.

Week 4**:** Postulates of quantum mechanics. Introduction to operator algebra.

Week 5**:** Origin of quantization: Particle in a box, particle in a ring.

Week 6**:** Hydrogen atom.

Week 7**:** Atomic orbitals. Orbital approximation and its limitation. Effective nuclear charge.

Week 8**:** Introduction to spin. Slater determinants. Self consistent fields.

Week 9**:** Valence bond and molecular orbital theories. Molecular orbitals of homonuclear and heteronuclear diatomic molecules.

Week 10**:** VSEPR. Molecular orbital and Valence bond approaches to polyatomic molecules. Hybrid orbitals.

Week 11**:** Huckel theory.

Week 12**:** Introduction to approximation methods. Scope of further study.