

CONCEPTS OF CHEMISTRY FOR ENGINEERING

MULTI-FACULTY

INTENDED AUDIENCE : Any Interested Learners

INDUSTRIES APPLICABLE TO : L&T power

COURSE OUTLINE :

This course is specifically designed for the BTech/BE engineering students. An appropriate contribution from all the core areas of chemistry (physical, inorganic, and organic) has been assembled here to provide the students an in-depth understanding of the fundamental topics. Additionally, the course outline has been designed to ensure the exposure of the students to chemistry-related interdisciplinary topics that will aid the students later in their core subject areas.

ABOUT INSTRUCTOR :

Prof. Anindya Datta is a Professor of Chemistry in IIT Bombay, with research interest in ultrafast spectroscopy and time resolved fluorescence microscopy. I have teaching experience of 17 years. 14 Ph. D. students have graduated from our laboratory. Eight more are working towards their degree. I received Excellence in Teaching Award from our institute in 2017 and have taught two NPTEL courses: one on Molecular Spectroscopy and another on Symmetry in Chemistry.

Prof. Debabrata Maiti is an associate professor in the chemistry department, IIT Bombay. He is also playing the role of an associate editor of the journal of organic chemistry (JOC). He specializes in inorganic and organic chemistry.

Prof. Chidambar Kulkarni is an assistant professor in the chemistry department, IIT Bombay. He is a polymer chemist by training and teaches organic chemistry.

Prof. Arnab Dutta is an assistant professor in the chemistry department, IIT Bombay. His research interest lies in the field of bio-inorganic chemistry. He specializes in teaching the courses belongs to inorganic chemistry.

COURSE PLAN :

Week 1: Schrodinger equation; Particle in 1D box: Solutions and applications for conjugated molecules and nanoparticles; H-atom wave functions: plots and spatial variations; Molecular orbitals of diatomic molecules and plots of multicenter orbitals

Week 2: Equations for atomic and molecular orbitals; Energy level diagrams of diatomic molecules ; π -molecular orbitals of butadiene, benzene, and aromaticity

Week 3: Effective nuclear charge; penetration of orbitals; variations of s, p, d, and f orbital energies, electron affinity and electron negativity; Polarizability, oxidation states, coordination numbers, and geometries; hard soft acids and bases; Molecular geometries

Week-4: Chemical bonding and molecular symmetry; Crystal field theory

Week-5: Ligand field theory; Energy diagrams of transition metal ions and their magnetic properties; Band structures of solids and the role of doping on band structures

Week-6: Principles of spectroscopy and selection rules; Vibrational and rotational spectroscopy for diatomic molecules & Applications

Week-7: Fluorescence Spectroscopy and its application in medicine; Electronic Spectroscopy

Week-8: Nuclear magnetic resonance and magnetic resonance imaging; Surface characterization techniques

Week-9: Ionic, polar, van Der Waals interactions, Equation of state for real gases and critical phenomena; Potential energy surfaces of H₃, H₂F, HCN molecules and trajectories on surfaces

Week-10: Thermodynamic functions: Energy, entropy, and free energy; Estimations of entropy and free energies; Free energy and EMF; Cell potentials; Nernst equation and applications; Acid base, Oxidation reduction, and solubility equilibria; Use of free energy considerations in metallurgy through Ellingham diagrams

Week-11: Representations of three-dimensional structures; Structural isomers and stereoisomers; configuration and symmetry and chirality; enantiomers and diastereomers; Optical activity; absolute configurations and conformational analysis; Isomerism in transitional metal compounds

Week-12: Introduction to reactions involving substitution, addition, elimination, oxidation, reduction; Cyclization and ring openings; Synthesis of a commonly used drug molecule