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| **SCYA1102** | **ENGINEERING CHEMISTRY** | **L** | **T** | **P** | **Credits** | **Total Marks** |
| **3** | **1** | **0** | **3** | **100** |

**COURSE OBJECTIVES:**

* To understand the basic concepts of quantum chemistry for bonds to bands
* To learn the principles and applications of energy levels in molecules
* To explore the importance of functional materials for electronic devices
* To study the structure and properties of carbon materials
* To identify the significance of chemistry in engineering and technology

**UNIT 1 BONDS TO BANDS 9 Hrs.**

Introduction to quantum chemistry – Motion of a quantum mechanical particle in one dimension (time- independent) – Schrödinger wave equation for hydrogen atom (No derivation) – Physical meaning of wave function - Angular and radial wave functions and probability densities – Quantum numbers – Principal, azimuthal, spin and magnetic quantum numbers – Wave functions and orbital shapes - *s,p,d,f* - LCAO-MO of H2 – Band theory of solids: Conductors, semi-conductors and superconductors – Role of As and Ga doping on band structures.

**UNIT 2 MOLECULAR SPECTROSCOPY 9 Hrs.**

Electromagnetic spectrum – Interaction of radiation with matter – Energy levels in molecules – Microwave spectroscopy – Principle – Classification of molecules based on moment of Inertia – Rotational energy expression (J levels) – Calculation of J for CO molecule – Vibrational spectroscopy – Normal modes of vibrations – Vibrations of polyatomic molecules (CO2 and H2O) – Determination of Force constant – Electronic transitions in organic molecules – Mathematical derivation of Beer- Lambert’s law – Stimulated Emission – Lasers in action – Excimer laser, Diode laser and Gas laser.

**UNIT 3 FUNCTIONAL MATERIALS 9 Hrs.**

Introduction to conducting polymers – Charge transport carriers: Exciton formation in organic solar cells and organic light emitting diodes (principle and working) – Conduction mechanism in polymers: Soliton, polaron and bipolaron formation in polyacetylene and polyaniline – Liquid crystals: Characteristic features and phases of liquid crystals – Liquid crystal displays.

**UNIT 4 CARBON MATERIALS FOR HEALTH, STEALTH AND ENERGY 9 Hrs.**

Introduction to carbon materials – Fullerenes – Production, properties and applications – VanderWaal’s solid – Structure ofgraphene, graphene oxide and reduced graphene oxide – Mechanical and electrical properties of graphene – Graphene based energy storage devices for space applications – Carbon nanotubes – Single-walled and multiwalled CNTs - Synthesis of CNTs by Thermal CVD and laser ablation method – Electrical and mechanical properties of CNTs - Applications of CNTs.

**UNIT 5 ENGINEERING MATERIALS 9 Hrs.**

**Phase equilibria:** Gibbs phase rule – Terms involved in Phase rule – Phase diagram of water system – Thermal method of analysis – Construction of simple eutectic system (Lead-Silver system).

**Fuels** – Classification of fuels – Determination of calorific values of solid fuels by bomb calorimeter – Manufacture of synthetic petrol by Fischer-Tropsch method – Knocking in IC engines – Chemical structure – Octane and cetane rating of fuels.

**Nanomaterials:** Size dependent properties of nanomaterials – Synthesis of gold and silver nanoparticles by Chemical reduction method – Applications of nanoparticles in medicine.

**TEXT / REFERENCE BOOKS**

1. A.K.Chandra, Introductory Quantum Chemistry, Tata McGraw-Hill, 4th edition, 1994.
2. Ira N. Levine, Physical chemistry, 6th Edition, 2008.
3. Ira N. Levine, Quantum chemistry, 7th Edition, 2013.
4. David W. Ball and Thomas Baer, Physical Chemistry, Wadsworth Cengage Learning, 2nd Edition, 2014.
5. Donald W. Rogers, Concise Physical Chemistry, John Wiley and Sons, 2011.
6. Douglas A. Skoog and Donald M.West, Principles of Instrumental Analysis, Cengage, 6th Edition, 2014.
7. P.C. Jain and Monika Jain, Engineering Chemistry, Dhanpat Rai Publication, 2018.
8. Joel. R. Fried, Polymer Science and Technology, Prentice Hall of India Private Ltd., 3rd Edition, 2012.