

UNIT-I Molecular Biophysics

Basic ideas on structure and conformation of simple molecules, structural features of proteins, nucleic acids, carbohydrates, and lipids. Aspects of biomolecular forces. Higher order structural organisation of proteins and nucleic acid, Basic thermodynamics, ligand binding and co-operativity in biological systems, kinetics, diffusion, and sedimentation.

UNIT-II Nanomaterials for Energy Conversion and Storage Materials

Nanomaterials for Solar Energy Conversion Systems. Principles of photovoltaic energy conversion (PV), Structural characteristics and concepts. Types of photovoltaic Cells, Physical concept of photovoltaic cells, Organic solar cells, Dye-Sensitized Solar Cells, Organic-Inorganic Hybrid solar cells. Device fabrication techniques and characterizations.

UNIT-III Computational Design on Drugs and Functional materials

Structure representation: Building of small molecules, co-ordinate system for structure representation, Building of Biopolymers and oligopeptides, Conformational analysis, Molecular Docking, Structure and features of conducting and semiconducting organic materials, Machine Learning approach as future prospect.

Text Books

1. Principles of Biochemistry: International Edition, David Nelson, and Michael Cox, WH Freeman; 7th ed. 2017
2. Biophysical Chemistry, Charles R. Cantor, and Paul R. Schimmel, W. H. Freeman, 1980
3. Organic Photovoltaics – Materials, Device Physics and Manufacturing Technologies, (eds. C. Brabec, V. Dyakonov, U. Scherf), 2nd Ed., Wiley-VCH, Germany, 2014.
4. Solar cells: Operating principles, technology and system applications by Martin A Green, Prentice Hall Inc, Englewood Cliffs, NJ, USA, 1981.
5. Introduction to Computational Chemistry by Frank Jensen, Wiley publication.
6. Andrew R. Leach, Molecular Modeling: Principles and Applications, 2nd Ed., Prentice Hall, 2001.