Value Added Courses

Department of Chemistry

Presidency University Kolkata

Department of Chemistry
(Faculty of Natural and Mathematical Sciences)
Presidency University
Hindoo College (1817-1855), Presidency College (1855-2010)
86/1, College Street, Kolkata - 700 073
West Bengal, India

Course CHEMVAC1: Sustainable Development

Odd Semester (30 hours)

Course Objective:To impart job-oriented skillsthrough hands-on experiment on water quality assessment and spectrophotometric detection of various water contaminant.

Part-1

Water Quality Analysis:

Theoretical principle of determination of Total Alkalinity of water, total hardness of the water sample, pH of ground and waste water, Dissolved oxygen of waste water, Chemical oxygen demand of waste water, salinity of the given water sample, turbidity of various water sample, detection and measurement of various contaminant using spectrophotometric methodsuch as nitrate, chloride, fluoride, iron, micro-pollutants.

LAB:

1. Measurement of total hardness of water.
2. pH measurement of ground water.
3. COD determination of water sample.

Reference Book:

1. Environmental Chemistry, (9^{th} ed.)-Anil K De.
2. Water Quality Concepts, Sampling, and Analyses-Y. Li, K. Migliaccio
3. Handbook of Methods In Environmental Studies, Vol.l Water and Wastewater Analysis-S. K. Maity

Course learning outcomes:

After the completion of the course, the students should be able to

1. Analize the ground and industrial waste water
2. Able to determine the common water contaminant using spectrophotometric technique

Even Semester (30 hours)

Course Objective:To impart job-oriented skillsthrough hands-on experiment on Chemical sensing of pollutant, Modern energy storage and conversion systems for sustainable development.

Part – 2

Chemical Sensing of Environmental Pollutant

Basic principle and designing of Chemical sensors. Synthesis and characterization methods. Development and making of in-house economical sensor kit for real time naked eye detection of various environmental pollutants.

Electrochemical Energy Storage and Conversion for Sustainable Developments

Classification of energy storage devices-batteries and supercapacitors; Energy storage mechanisms; Materials design for energy storage; Cyclic voltammetric and electrochemical impedance spectroscopic characterizations for energy materials.

LAB:

1. H_2S sensing using SALAN type metal complex

Reference Book:

1. Electrochemical Supercapacitors: Scientific Fundamentals and Technological Applications - B. E. Conway
2. Lithium-Ion Batteries: Science and Technologies -M. Yoshio, R. J. Brodd and A. Kozawa
3. Lead-Acid Batteries: Science and Technology - D. Pavlov
4. Environmental Chemistry, (9^{th} ed.), -Anil K De.

Course learning outcome:

After the completion of the course, the students should be able to

1. design chemical sensor
2. make sensor kit
3. Explain the fundamental concepts of batteries and supercapacitors
4. Design the optimized hybrid device based on the targeted application.

Course CHEMVAC2: Mathematical Tools and use of Application Software in Chemistry

Course Objectives: The course aims to impart analytical, numerical, computational and technical skills on the relevant field of Chemistry for facilitating employability in academia and industries

Odd Semester (30 hours)

Unit 1 (16 hours)

Mathematical Tools: Coordinate geometry: Cartesian and polar coordinate systems and their interconversion.

Preliminary idea about complex number and complex variable.

Vectors and Matrices: Vectors, preliminary idea of vector space, matrix algebra, matrix inversion, matrix eigenvalue and eigenvector, solution of simultaneous algebraic equation with more than two unknowns.

Elementary analytical methods to solve differential equations.

Functional Series and Integral Transforms: Fourier transform, Laplace transform.

Power series method for differential equations (Hermite, Legendre, Laguerre differential equations)

Unit 2 (10 hours)

Mathematica and Matlab: Introduction to Mathematica and Matlab for symbolic computation of simple algebra and numerical mathematics.

Evaluating and plotting mathematical functions, solving algebraic equations, solving simultaneous equations, differentiation, integration, integral transform, series, solving differential equations (ODE & PDE), performing matrix algebra, curve fitting.

Unit 3 (4 hours)

LATEX: Introduction of LATEX, downloading and installing TeXstudio or TeXmaker, writing equations, making tables, inserting figures and references.

JabRef: Managing and citing references in LATEX typesetting system.

Course learning outcome: After the completion of the course, the students should be able to

1. Perform analytical calculations of the mathematics involved in the elementary physical chemistry.
2. Use Mathematica and Matlabsoftwares to perform algebraic and numerical calculation and visualize mathematical functions by plotting graphs relevant to the topics of physical chemistry like chemical kinetics, thermodynamics, quantum chemistry etc.
3. Write scientific documents using the typesetting platform LATEX.

Even Semester (30 hours)

Unit 4 (5 hours)

Origin and SciDAVis: Introduction of origin and SciDAVis, GNU plot, drawing various 2D & 3D plots, data analysis, statistics, signal processing, curve fitting, peak analysis, conversion of graph to various file format like JPEG,GIF,EPS.

Unit 5 (4 hours):

ChemDraw and ChemSketch: Introduction of ChemDraw, chemical name to structure conversion, chemical structure to name conversion, mass spectrum simulation, NMR spectrum simulation (both ^{1}H NMR &^{13}C NMR), structure clean up, 3D chemical structure, export to SVG,PDF, TIFF.

Introduction to ChemSketch, molecular modelling, creating and modifying images of chemical structures, writing and performing chemical equations and diagrams.

Unit 6 (16 hours)

Use of application software such as Gaussian, Turbomole, ORCA, AutoDock, Schroidinger Suite andChemCraft in chemistry:

- Energy minimization, structure optimization, calculating analytical frequency.
- Transition state optimization, comparison of rate constants.
- Thermochemistry.
- Calculating IR, UV, NMR, VCD spectra of small molecules.
- MO analysis, population analysis (NBO).
- Molecular Docking (Protein-ligand) for drug design.

Unit 7 (5 hours)

Mercury, ORTEP, CSD(CCDC): Three dimensional visualization of X-ray crystal structure of organic and inorganic compounds, exploration of crystal packing in unit cell, H-bonding interaction.

Zotero and Mendeley: Managing references and citations.

Course learning outcome: After the completion of the course, the students should be able to

1. Use of software relevant to chemistry, scientific graph plotting and data analysis.
2. Apply ChemDraw and ChemSketchsoftware for molecular modelling, writing structures and chemical equations.
3. Operate various Quantum Chemical and Docking software, analyze and interpret the results obtained by calculation to rationalize experimental outcomes or even making testable prediction.
4. Understand the crystal structure and bonding in molecule. They would learn to organize references in an article.