DEPARTMENT OF CHEMISTRY

MANONMANIAM SUNDARANAR UNIVERSITY, TIRUNELVELI-12

Ph.D. Course Work Papers

Sl. No.	Name of the Course	Credit
1	Analytical Methods And Instrumentation	4
2	Corrosion Science and Engineering	4
3	Research and Teaching Methodology	4
4	Advanced Scientific Techniques in Chemical Analysis	4
5	Advanced Topics in Organic Chemistry	4
6	Chromatography	4
7	Advanced Topics in Physical Chemistry	4
8	Adsorption and Catalysis	4
9	Nanomaterials And Their Applications To Solar Energy Conversion	4
10	Phyto-Biosynthesis and Applications of Metal Nanoparticles	4
11	Mini Project	4
12	Heterogenous Catalysis	4

Paper: I

ANALYTICAL METHODS AND INSTRUMENTATION

Hrs.– 60 **Credit – 4**

Objectives:

1. To understand the analytical data interpretation and result analysis.
2. To study about various chromatography technique for chemical analysis.
3. To study about the spectroscopic technique and instrumentation method of chemical analysis.

Unit-I Treatment of Analytical data and Interpretation (12hrs.)

Accuracy and Precision in measurements. Reliability of Analytical Data – Errors in Chemical analysis, Classification, Determination. Improving accuracy of analysis. Statistical analysis – Student t-test, F-test.

Unit-II Separation Technique (12hrs.)

Chromatographic techniques – paper, thin layer column chromatography, Gas Chromatography (GC)- Instrumentation, application. Principle and application of GCMS, LCMS, ion exchange chromatography. Flash Chromatography (FC) – Principle and application. Extraction Methods – Solvent extraction, Solid Phase extraction (SPE). Microwave Assisted Extraction (MAE), Soxhlet Extraction.

Unit- III Instrumental Methods of Chemical Analysis (12hrs.)

Atomic Absorption Spectroscopy (AAS) and Atomic Emision Spectroscopy (AES) – Principle Instrumentation and Application. X-ray Photoelectron Spectroscopy (XPS) – Theory and Instrumentation, XPS imaging, Surface analytical techniques – XRD, SEM, TEM – applications.

Unit-IV Spectroscopic Analysis (12hrs.)

UV-Vis and IR spectroscopy – UV-Vis spectra of enes, enones, arenes, and conjugated systems. Effect of solvent on UV-Vis spectra. IR- Principle, Instrumentation and Application. Characteristiiic group frequencies and functional group detection using IR.

Mass Spectroscopy (MS) – EI, CI, FAB, ESI and MALDI ion sources. Characteristic EIMS fragmentation and MS rearrangements. Spectral interpretation and structural determining using mass spectrum.

Unit-V NMR Spectroscopy and Structure elucidation (12hrs.)

Basic Principle of NMR $-H^1$ and C^{13} Chemical Shift, spin-spin coupling, Coupling constant, J-value. Applications of NOE, DEPT and 2D techniques – COSY, HSQC and HSBC. Structure elucidation of organic compounds using spectral data – UV, IR, NMR and MS.

References:

1. Douglas A. Skoog. F James Holler; Stanley; R. Cruch, "Principle of instrumental analysis" Cole pub Co, (2006).
2. S.M. Khopkar, " Basic Principles of Analytical Chemistry" 1st Edition, Wiley pub, (1984).
3. W. Kemp, "Organic Spectroscopy", 3rd Edition, Palgrave Macmillan, (1991).
4. D.L. Pavia, G.M. Lampman and G.S. Kriz " Introduction to Spectroscopy" 3rd Edition, Brooks/Cole, (2001).
5. D.H. Williams and I. Fleming " Spectroscopic Methods in Organic Chemistry" 5th Edition, Macraw-Hill (1989).

Paper: II

CORROSION SCIENCE AND ENGINEERING

Hours : 60 **Credits: 4**

Objectives

1. To study the Principle and mechanism of electrochemical reactions involved in corrosion and preventive methods.

2. To gain knowledge on measurement of various adsorption and thermodynamic parameters related to corrosion.

3. To learn the basic terminology involved in electrochemical cell reaction and their application in some electrochemical based titration.

4. To understand the principles and working of some batteries and fuel cells. To impart knowledge on Classification, properties and uses of alloys.

5. To study the preparation, properties and applications of engineering materials.

Unit-1: Corrosion (12 hrs)

Definition – causes - factors – types – chemical, electrochemical corrosion (galvanic, differential aeration), corrosion control – material selection and design aspect – electrochemical protection – sacrificial anode method and impressed current cathodic method. Paints – constituent and function, Electroplating of copper and electroless plating of nickel

Unit-II: Non-Electrochemical methods (12 hrs)

Adsorption - Physisorption – Chemisorption - Surface area determination - Mass loss measurements, Corrosion parameters Temperature studies – Adsorption - Temkin – Langmuir adsorption isotherm, Change in entropy, enthalpy, Gibbs free energy, Heat of adsorption, Activation energy - Green inhibitors.

Unit-III: Electrochemistry **(12 hrs)**

Electrochemical cell – redox reaction, electrode potential – origin of electrode potential – oxidation potential – reduction potential – electrochemical series and its significance – Nernst equation. Precipitation titration - Conductometric titration – Potentiometric titration – pH meter.

Unit-IV: Batteries, Fuel cells and Alloys **(12 hrs)**

Batteries - Types of batteries – alkaline battery – lead storage battery – nickel cadmium battery – lithium battery – Fuel cells – Hydrogen oxygen fuel cell.

Alloys: Introduction – Definition – Properties of alloys – Significance of alloying, Function and effects of alloying elements – Ferrous alloys – Nichrome and Stainless steel – heat treatment of steel; Non-ferrous alloys – brass and bronze.

Unit-V: Engineering Materials **(12 hrs)**

Abrasives: definition, classification or types, grinding wheel, abrasive paper and cloth.

Refractories: definition, characteristics, classification properties – refractoriness and RUL, dimensional stability, thermal spalling, thermal expansion, porosity: Manufacture of alumina, magnesite and silicon carbide.

Reference:

1. R. Winston Revie and Herbert H. Uhlig "Corrosion and Corrosion control: An introduction to Corrosion Science and Engineering", 4th Edition, John Wiley & Sons, Inc, 2008
2. Perez, Nestor "Electrochemistry and Corrosion Science", 2nd Edition, Springer
3. Principles of Materials Science & Engineering, 2nd Edition by W. F. Smith, 1990
4. Robert G. Kelly, John R. Scully, David Shoesmith, Rudolph G. Buchheit **"**Electrochemical Techniques in Corrosion Science and Engineering" 1st Edition, 2002
5. Volkan Cicek, Bayan Al-Numan "Corrosion Chemistry" Wiley
6. Pierre R. Roberge, "Handbook of Corrosion Engineering", McGraw-Hill, 2005

7. B. Siva Shankar, “Engineering Chemistry”, Tata Mc Graw Hill Publishing Limited, 3rd Edition, 2015.
8. S. S. Dara, Mukkanti, “Text of Engineering Chemistry”, S. Chand & Co, New Delhi, 12th Edition, 2006.
9. C. V. Agarwal, C. P. Murthy, A. Naidu, “Chemistry of Engineering Materials”, Wiley India, 5th Edition, 2013.
10. R. P. Mani, K. N. Mishra, “Chemistry of Engineering Materials”, Cengage Learning, 3rd Edition, 2015.
11. S.L.Chawla, R.K.Gupta, “Materials selection for corrosion control, First printing, Dec.1993.
12. P.H.Reiger, “Electrochemistry”, Prentice Hall, 1987.
13. Mars G. Fontana, Corrosion Engineering, McGraw Hill Education, 3rd Edition
14. S. Glasstone, An introduction to Electrochemistry, Van Nostrand, New York, 1965.
15. A. J. Bard, L.R. Faulkner, Electrochemical Methods: Fundamentals and Applications,John Wiley and Sons, New York, 1980.
16. R. Crow, Principles and Applications of Electrochemistry, Chapman and Hall, London,1979.
17. J. D. M. Bockris, A.K.N. Reddy, Modern Electrochemistry, Vol. I & II, Plenum Press,New York, 3rd Reprint, 1977.
18. Dr.A.Ravikrishnan, “ Engineering chemistry – II” , Sri Krishna Hitech Publishing Company Pvt.Ltd, Updated edition,2015-2016.
19. Dr.A.Ravikrishnan, “ Engineering chemistry ” , Sri Krishna Hitech Publishing Company Pvt.Ltd, Revised edition,2017-2018.
20. P. C. Jain, Monica Jain, “Engineering Chemistry”, Dhanpat Rai Publishing Company, 15th Edition, 2015.
21. Shasi Chawla, “Text Book of Engineering Chemistry”, Dhantpat Rai Publishing Company, New Delhi, 1st Edition.
22. Dr. V. Veeraiyan and Dr. L. Devaraj Stephen, “ Engineering chemistry – II” VRS Publishers Pvt.Ltd, 2015-2016.

Paper-III

RESEARCH AND TEACHING METHODOLOGY

No. of Hrs – 4 / Week **Credits - 4**

Objective

1. *To introduce the purpose and importance of research for future development.*
2. *To know the various indexes and abstracts in science and technology as a source of all information in chemistry.*
3. *To learn the ways of carrying out literature search for current awareness and for the retrospective survey.*
4. *To know the methodology of writing thesis and journal articles.*
5. *To know about the teaching methodology for teaching the scientific concepts and techniques to students*

Unit –I : Scientific Research **(12hrs.)**

Introduction to Research, Selection of a research topic, reviewing the literature, preparing the proposal and design of study Experimentation and interpretation of results. Formation, testing and rejection of hypothesis. Preparation and presentation of reports, dissertation and thesis writing.

Unit-II : Chemical Literature **(12hrs.)**

Primary and secondary literature: Journals, Patents, Reviews, Chemical abstracts, treatises, monographs and online journals. Web browsing for Research. ASAP alerts, CA Alerts, Scifinder, Chemport, Science direct, STN international, Journal home pages. **Impact factor, citations and h-index. Scopus, Web of Science and Google scholar.**

Unit-III: Error Analysis **(12hrs.)**

Limitation of analytical methods, accuracy, precision & minimization of errors – systematic and random errors and reliability of results – Mode – Median – Mean – Standard deviation- Variance & Covariance, normal distribution and the normal probability curve.

Unit-IV: Correlation methods & Non-parametric tests (12hrs.)

Scatter diagram and linear regression line: Spearman rank order correlation, Pearson's product moment correlation - Correlation co-efficient.

Non-parametric tests - χ^2 test, Median test, Mann-Whitney test, Sign test, Wilcox on matched-pairs signed ranks test.

Unit-V: Methodology of Teaching (12hrs.)

Teaching- Objectives of Teaching, Phases of Teaching – Teaching methods: Lecture Method, Discussion Method, Discovery Learning, Inquiry, Problem Solving Method, Project method, Seminar – Integrating ICT in Teaching: Individualized Instruction, Ways for Effective Presentation with Power Point- Documentation – Evaluation: Formative, Summative & Continuous and comprehensive Evaluation- Later Adolescent Psychology: Meaning, Physical, Cognitive, Emotional, Social and Moral Development – Teaching Later Adolescents

References:

1. Rajammal P. Devadas, A Handbook of Methodology of Research, S.R.K. Vidyalaya Press, Chennai, 1976.
2. J. Anderson, B.H. Durstan and M. Poole, Thesis and assignment writing, Wiley Eastern, New Delhi, 1977.
3. R.O. Butlet, Preparing thesis and other manuscript.
4. R. L. Dominoswki, *Research Methods*, Prentice Hall, 1981.
5. J. W.Best, *Research in Education*, 4th ed. Prentice Hall of India, New Delhi, 1981.
6. H. F. Ebel, C. Bliefert and W.E. Russey, *The Art of Scientific Writing*, VCH, Weinheim, 1988.
7. Joseph, A. *Methodology for Research*; Theological Publications: Bangalore, 1986.
8. Sampath, K., Panneerselvam, A. & Santhanam, S. (1984). Introduction to educational technology. (2nd revised ed.). New Delhi: Sterling Publishers.
9. Sharma, S.R. (2003). Effective classroom teaching modern methods, tools & Techniques. Jaipur: Mangal Deep
10. Vedanayagam, E.G. (1989). Teaching technology for college teachers. New York: Sterling Publishers.

Paper-IV

ADVANCED SCIENTIFIC TECHNIQUES IN CHEMICAL ANALYSIS

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To master the basic principles of spectroscopy to apply for structural elucidation.*
2. *To learn the methods of characterizing compounds by spectroscopic techniques.*
3. *To learn the various instrumental methods studying a given compound.*
4. *To learn the separation techniques for organic and inorganic compounds.*
5. *To learn about industrial analytical processes.*

Unit –I : Absorption Spectroscopy (12hrs.)

Infrared and Raman Spectroscopy: FT-IR, basic principles, quantitative IR, resonance Raman and laser Raman spectroscopy, applications of IR and Raman spectroscopy to organic and inorganic compounds.

Electronic Spectroscopy: term symbols, spin-orbit coupling in free ions, electronic spectra of O_h and T_d complexes, charge transfer transition, structural evidence from electronic spectra.

Unit II: Applications of Advanced Organic Spectroscopy (12hrs.)

NMR: Basic principles of two-dimensional NMR spectroscopy – HOMOCOSY, HETCOSY and NOESY spectra and their applications – use of INEPT and DEPT methods and their applications.

Mass: Molecular ions, isotope peaks, fragmentation pattern – McLafferty rearrangement - measurement techniques (EI, CI FI, FD, FAB, SIMS, MALDI) – M^{+1} and M^{+2} ions – calculation of molecular formula from P_{M+1} and P_{M+2}

Road-map problems covering UV, IR, ^{1}H-NMR, ^{13}C-NMR and mass spectral data.

Unit-III: Spectroscopy (12hrs.)

Nuclear Quadruple Resonance Spectroscopy: effect of magnetic field on the spectra, electric field gradient and molecular structure, structural elucidation of inorganic and coordination compounds.

Electron Paramagnetic Resonance Spectroscopy: hyperfine splitting in isotropic systems; epr spectra of systems with more than one unpaired electrons-Kramer's degeneracy, zero field

splitting, epr of triplet states, anisotropy in *g*-value, anisotropy in hyperfine splitting, nuclear quadrupleinteraction; applications of epr to organic and inorganic compounds.

Mossbauer Spectroscopy: interpretation of isomer shifts, quadruple and magnetic interactions, Mossbauer emission spectroscopy, structural elucidation.

Unit IV: Diffraction & Surface Techniques: (12hrs.)

Principles and applications of XRD, Neutron and electron diffraction – Scanning electron microscopy (SEM)- Instrumentation – applications – surface area analysis, particle size determination – Scanning Probe Microscopes – Scanning Tunneling Microscopes – Atomic force microscopes (AFM) – Principle &applications.

Unit V: Electrochemical Techniques (12hrs.)

Polarography – Chronopotentiometry – Chronoamperometry – chronocontometry- Linear Potential Sweep voltametry – Cyclic Voltametry – ImpendenceMeasurements – AC Voltametry – Principles and their applications.

References:

1. Introduction to Nanoscience- Gabor. L, Hornyak. Joydeep Dutta CRC Press 2008.
2. L. Antropov, Theoretical Electrochemistry, Mir Publication, Moscow, 1972.
3. D.A. Skoog and J.J. Leary, Principles of Instrumental Analysis, 4th Edn., Saunders College Publishing, 1992.
4. D.A. Skoog, F.S.Holler, S.R.Crouch, Principles of Instrumental Analysis, 6th Edn., Thomson Brooks/cole, 2007.
5. A.K. Cheetham, P.Day, Solid State Chemistry: Techniques, Oxford University Press, Oxford, 1987.
6. G. E. Bacon, Neutron diffraction, Oxford Universtiy Press, Oxford, 1975.
7. R.S. Drago, Physical Methods in Chemistry, Saunders, 1999.
8. Spectrometric Identification of Organic Comounds – Silverstein, Bassler and Morril.
9. Organic Spectroscopy – William Kemp

Paper V

ADVANCED TOPICS IN ORGANIC CHEMISTRY

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To learn the various reagents and their application in organic synthesis*
2. *To study the retro synthetic analysis*
3. *To understand the concept of linear free-energy relationships*
4. *To know about the biochemical activities of amino acids and proteins*
5. *To study on the nucleic acids structure and function*

Unit I: Organic Reagents (12hrs.)

Gilman's reagents – DCC – Grignard reagents – crown ethers – NBS – BF_3 complexes – SeO_2 – 1, 3-dithiane, tri-n-butyl tin hydride – phase transfer catalysts – Wilkinson's catalyst.

Unit II: Retro synthetic Analysis (12hrs.)

Introduction to disconnections – one group disconnections – two group disconnections – peri cyclic reactions – Heteroatoms and heterocyclic compounds – small rings: three membered, four membered, and five membered.

Unit III: Advances in Linear Free-Energy Relationships (12hrs.)

An introduction to linear free-energy relationships (LFER) – the Hammett equation – the duality of substituent constants and the Yukawa-Tasumo equation – the general validity of the Hammett equation – deviations from the Hammett equation in its various forms; the separation of polar, steric and resonance effects – Taft's equations; the ortho-effect; application of LFER to organic reactions; Influence of solvent on organic reactivity; the reactivity-selectivity principle.

UNIT IV: **Amino Acids and Proteins (12hrs.)**

Structure and Classification – abbreviated names (1 letter and 3 letter) – Physical properties of amino acids – chemical properties – codons – Structure and importance of simple peptides like glutathione, Carnosine, anserine, vasopressin – Peptide antibiotics – gramicidin,

bacitracine, actinomycin D - Peptide synthesis – Acid chloride method – DCC method – Determination of primary structure of peptide – Identification of N-terminal amino acid – Barger's method – the DNP method – identification of C-terminal amino acid – Hierarchial representation of protein Primary, Secondary, tertiary and quaternary structures – Ramachandran plot.

UNIT V: Purine, Pyrimidine and Nucleic Acids (12hrs.)

Structure of Purines, Pyrimidines – Nucleoside – ribonucleoside, deoxyribonucleosides – nucleotides – ribonucleotides – deoxyribonucleotides – structure and functions of DNA - Watson and Crick model of DNA- Structure of types of RNA (m-RNA, t-RNA and r-RNA) – Nucleases – structure and function of DNA and RNA – polynucleotide – cyclic nucleotide – structure and function of cAMP, cGMP nucleoprotein – Types of DNA (A-DNA, B-DNA, Z-DNA)

References:

1. Reaction Mechanism and Reagents in Organic Chemistry – Gurdeep R. Chatwal
2. Designing Organic Synthesis: A Programmed Introduction to the Synthon Approach – Stuart Warren
3. N.B. Chapman and J. Shorter, Eds., Advances in Linear Free-Energy Relationships, Plenum Press, London, 1972.
4. J. Shorter, Correlation Analysis in Organic Chemistry – An Introduction to Linear Free-Energy Relationships, Clarendon Press, Oxford, 1973.
5. N.B. Chapman and J. Shorter, Eds., Correlation Analysis in Chemistry-Recent Advances, Plenum Press, New York, 1978.
6. J. Shorter, Correlation Analysis of Organic Reactivity, Research Studies Press, England, 1982.
7. Biochemistry, Lehinger J.CB S.Publishers,1993.
8. Biochemistry, U. Satyanarayana & U. Chakrapani, Books & Allied Pvt. Ltd, 1999.
9. Biochemistry — Lubert Stryer – W. H. Freeman and company, 4th Edn., New York, 1995.

Paper VI

CHROMATOGRAPHY

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To understand the chromatographic basic principles*
2. *To learn the thinlayer chromatographic techniques*
3. *To understand about the ion exchange concepts*
4. *To learn about the high performance liquid chromatography for organic analysis*
5. *To study about the gas chromatography technique for volatile and gas molecule analysis*

UNIT I: Chromatography (12hrs.)

Classification of Chromatography methods. Column Chromatography- Principles, experimental procedures, stationary and mobile phases, Choice of Solvent Systems, Separation techniques. Applications.

R_f values, Factors affecting R_f values, Experimental procedures, Choice of paper and solvent systems, developments of chromatogram. Detection of the spots. Ascending, Descending and Radial Paper Chromatography, Two Dimensional Chromatography –Applications**.**

UNIT II: THINLAYER CHROMATOGRAPHY (12hrs.)

Principles, factors affecting R_f values. Experimental Procedures, Choice of adsorbents and Solvents. Preparation of plates, development of the Chromatogram. Detection of the spots, advantages of thin Layer Chromatography over paper chromatography and Applications.

UNIT III: ION EXCHANGE CHROMATOGRAPHY (12hrs.)

Principle, ion exchange resins and their types- cation exchange resins, anion exchange resins, ion exchange equilibria, properties of ion exchange resins, ion exchange capacity and techniques – applications.

UNIT IV: HIGH PERFORMANCE LIQUID CHROMATOGRAPHY (12hrs.)

Introduction, instrumentation, stationary and mobile Phases. Mobile Phase – Composition. Column – Preparation, Cleaning –regeneration and Storage Conditions. Retention time- Types of HPLC. Applications.

UNIT V: GAS CHROMATOGRAPHY (12hrs.)

Principle, instrumentation choice of injectors, column and detectors - Programmed temperature chromatography, flow programming chromatography, gas-solid chromatography, and hyphenated techniques in chromatography- Applications of Gas chromatography.

REFERENCES:

1. Fundamentals of Analytical Chemistry – D.A.Skoog, D.M. West, F.J. Holler and S.R. Crouch – 2004; Thompson Asia Private Ltd., Bangalore.
2. Instrumental Methods of Analysis – B. K. Sharma, 2003; Goel publishing House, Meerut.
3. Contemporary Chemical Analysis - Judith F. Rubinson, Prentice Hall (India).
4. Instrumental Methods of Analysis Hobart H. Willard, Lynne L. Merritt Jr, John Dean, Wadsworth Publishing Co Inc; 7th Edn., 1988.
5. Thin Layer Chromatography- A laboratory Handbook, Ashworth, Stahl. E., 1st Edn., Springer-Verlag, 1969.
6. Dynamics of Chromatography - Principles and Theory, J. Calvin Giddings, CRC Press, 2002.
7. Principles of Instrumental Analysis, Douglas A. Skoog, F. James Holler, Stanley R. Crouch, 2006.

Paper VII

ADVANCED TOPICS IN PHYSICAL CHEMISTRY

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To study about the concept of Photochemistry*
2. *To understand the principles about the chemical kinetics*
3. *To learn about the thermodynamics behavior of systems in chemistry*
4. *To understand the physical characteristics of biomolecules*
5. *To understand the various concept of Analytical techniques*

Unit I: Advanced Photochemistry (12hrs.)

Artificial photosynthesis and solar energy conversion – Photo electrochemical cells – dynamics of excited state processes (excited state energy, redox properties, emission lifetime and its temperature dependence) in micelles, reverse micelles and biomembranes – Fluorescence – quenching and anisotropy concepts; fluorescence sensing – mechanism and applications; Radioactive decay engineering – metal-enhanced fluorescence and surface Plasmon-coupled emission.

Unit – II: Advanced chemical kinetics (12hrs.)

Experimental methods for fast reactions- temperature jump, pressure jump stopped flow and flash photolysis – pulse technique – short tube kinetics.

NMR studies in rate process - Enzyme kinetics of complicated systems – theory of diffusion controlled reactions.

Unit – III: Irreversible thermodynamics (12hrs.)

Internal heat & entropy production – relation of entropy production with flux & forces – phenomenological equation – Prigogine's principle of minimum entropy production at non-equilibrium stationary state.

Unit – IV: Biophysical chemistry (12hrs.)

Biomembranes (structure & function) – Active transport & passive transport – multiple equilibria – specific examples of multiple equilibria – Transport processes – general features of transport processes optical systems of rht e study of transport processes – self organizing systems

– (Micelles, lipids, cyclodextrins, liquid crystals, reverse micelles) their interactions and solutions properties.

Unit – V: Analytical techniques (12hrs.)

Thermal methods: TGA, DTA, DSC, Thermometric titration - Adsorption/desorption techniques: BET and EGME methods of determination of external and total surface area.

References:

1. K. Kalyanasundaram, Photochemistry in Microheterogeneous Systems, Academic Press, Orlando, 1987.
2. Extended irreversible thermodynamics – David Jon, Jose casas Vazques, 2012
3. Understanding Non-equilibrium Thermodyanmics – Geogy Lebon, David Jon- 02008
4. Chemical kinetics: Fundementals & New developments, E.T. Densov, Ergenii tinofeerich , 2003
5. Chemical Kinetics, Laidler
6. Biophysical chemistry Alan Cooper – 2011
7. Biophysical chemistry, James P. Allen – 2008
8. Fundamentals of Analytical chemistry – Douglas A. Skoog Donal M. west 2013

Paper VIII

ADSORPTION AND CATALYSIS

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To study about the various adsorption process connected with catalysis process*
2. *To study about the preparation methods of adsorbents*
3. *To evaluate the physico chemical properties of adsorbent by spectral studies*
4. *To study about the vapour phase and liquid phase catalysis and adsorption parameters*
5. *To learn about the adsorption isotherms and product analysis*

Unit: I Adsorption & Catalysis (12hrs.)

Concept of adsorption – types of adsorption, monolayer and multilayer adsorption. Adsorption - activation energy and temperature relationships, different between adsorption and catalysis, catalysis - homogeneous catalysis, heterogeneous catalysis, Acid -- base catalysis.

Unit: II Methods of preparation (12hrs.)

Adsorbent - adsorbent preparation from plant materials, activated carbon preparation, synthetic adsorbent/catalyst - Molecular sieves – microporous & mesoporous molecular sieves – silicates, Aluminosilicates, Aluminophosphates – structure, acidic and basic sites.

Unit: III Spectral studies on Adsorbent (12hrs.)

Characterization of adsorbent and catalyst - X-Ray Diffraction (XRD), Fourier transform infrared spectroscopy (FT-IR), Differential thermal analysis(DTA) , Nuclear magnetic resonance spectroscopy (NMR), Temperature programmed desorption (TPD), Electron spin resonance spectroscopy(ESR) Scanning electron microscopy(SEM), BET Surface Area, pore size analysis.

Unit: IV Reactions & Factors (12hrs.)

Liquid phase - heterogeneous reaction conditions optimization - Temperature, pH, time and molar ratios. Vapor phase reaction, Regeneration of catalyst.

Adsorption – adsorption of dye molecules, metal ions, sugar molecules and other suitable molecules, conditions optimization – time, temperature, p^H, concentration and adsorbent dosage.

Unit: V Techniques (12hrs.)

Product analysis in catalysis reactions – Gas chromatographic technique, conversion and product selectivity.Interpretation of adsorption parameters - Adsorption kinetics, adsorption isotherms and adsorption thermodynamics.

References:

1. Environmentally stable adsorbent of tetrahedral silica and non tetrahedral alumina for removal and recovery of malachite green dye from aqueous solution, *J.Hazardous materials*, 157 (2008) 137-145.
2. Plant poisoning organic dyes adsorption on tomato plant root and green carbon from aqueous solution, *Desalination*, 249 (2009)1132-1138.
3. Film and pore diffusion modeling for the adsorption of direct red 81 on activated carbon prepared from balsamodendron caudatum wood waste, *Digest Journal of Nanomaterials and Biostructures*, Vol. 5, No 3, July 2010, p. 911 – 919
4. Plant toxic and non-toxic nature of organic dyes through adsorption mechanism on cellulose surface, *Journal of Hazardous materials*,189 (2011) 294–300.
5. Adsorption of cationic and anionic organic dyes from aqueous solution using Silica, *J. Environmental Science and Engineering*, volume 52, No.4 **(2010)** 361-366
6. Hazardous dyes removal from aqueous solution over mesoporous aluminophosphate molecular sieves with textural porosity by adsorption, Journal of Hazardous Materials 244– 245 (**2013**) 10– 20.
7. A Simple Method for the Synthesis of Thermally Stable Large Pore Mesoporous Aluminophosphate Molecular Sieves, Materials letters, 113 (**2013**) 93–95.
8. Aniline methylation over AFI and AEL type molecular sieves, *App. Catal*., Vol. 174, **1998**, 213.
9. Adsorptive removal of metanyl yellow on mesoporous Nickel aluminophosphate molecular sieves from aqueous solution, Asian J. of chemistry, vol. 24, no.12(2012), 5775-5778
10. Recent trends in catalysis**,** Narosa publication, 1st edition 2000.

Paper IX

NANOMATERIALS AND THEIR APPLICATIONS TO SOLAR ENERGY CONVERSION

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To study about the Nanomaterials*
2. *To study about the dye-sensitized solar cells*
3. *To learn about the Semiconductor and microemulsion (quantum dots)*
4. *To understand the Photochemistry and corrosion principles*
5. *To understand about the solar cell concepts*

Unit I: Nanomaterials (12hrs.)

Introduction to Nanoscience: Introduction- definition of Nanoscience, nanochemistry- classification of the nanomaterials

Synthesis of nanomaterials: Precipitative methods – hydrothermal and solvothermal methods - chemical methods - reduction methods – colloidal and micellar approach – sol-gel method – chemical vapor deposition method.

Specialized Nanomaterials: Metal oxide nanoparticles, semiconductor nanoparticles and core/shell nanoparticles

Unit II: Dye-sensitized solar cells (12hrs.)

Solar energy conversion and storage – photo electrochemical cells – dye-sensitized solar cells – design and fabrication - power conversion efficiency

Use of metal and metal-free dye sensitizers in photovoltaic devices.

Unit III: Semiconductor and microemulsion (quantum dots) (12hrs.)

Review of published literature – Water-soluble silica-coated semiconductor quantum dots – synthesis, characterization and properties.

Thickness-controllable silica coating of quantum dots – synthesis by microemulsion method and application in the growth of rice.

Unit IV: Photochemistry and corrosion (12hrs.)

Review of published literature – Silica coated cadmium sulfide nanocomposites – synthesis, structure, optic and its photo catalytic properties.

Zirconia-coated carbonyl iron particles – synthesis and corrosion study.

Unit V : Solar cell **(12hrs.)**

Review of published literature – Ruthenium (II) sensitizer in dye-sensitized solar cells using an organic dye as co-sensitizer – Fabrication and device characterization - photovoltaic performance.

Dye-sensitized solar cells - Co-sensitization strategy – electrochemical properties – Photo electrochemical performances – Electrochemical impedance spectroscopy – dark current measurement – Open-circuit voltage decay.

References

1. H. R. Allcock, Introduction to Materials Chemistry, John Wiley & Sons, Inc. Publication, 2008.
2. T. Pradeep, Nano: The Essentials, Tata Mc Graw-Hill, 2007.
3. A. Hagfeldt, *et al.* Chem. Rev., 2010, 110, pp. 6595–6663.
4. J. Gong, J. Liang, K. Sumathy, Renewable and Sustainable Energy Reviews, 2012, 16, 8, 5848-5860.
5. X. Chen, F. Liu, Q. Jiang, L. Sun, Q. Wang, J. Inorg. Organomet. Polym, 2012, 22:6-11.
6. A. Wang, Y. Zheng, F. Peng, J. Spectros. 2014, Article ID 169245, 1-5.
7. N. Gupta, B. Pal, J. Colloid and Int. Sci., 2010, 368, 250-256.
8. R. Chen et al. J. Colloid and Int. Sci., 2010, 342, 49-56.
9. U. Mehmood, I. A. Hussein, K. Harrabi, N. Tabet, G. R. Berdiyorov, RSC Adv., 2016, 6, 7897-7901.
10. L. Wei, Y. Na, Y. Yang, R. Fan, P. Wang, L. Li, Phys. Chem. Chem. Phys., 2015, 17, 1273-1280.

Paper X

PHYTO-BIOSYNTHESIS AND APPLICATIONS OF METAL NANOPARTICLES

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. *To study about the Extraction and Isolation of natural products from Medicinal plants*
2. *To synthesis nanomaterial by using natural products*
3. *To understand the physico chemical properties of Nanoparticles*
4. *To utilize the nanoparticles for Biological Applications*
5. *To study the Nanoparticles application on Green catalysis*

Unit I - Extraction and Isolation of some Indian Medicinal plants (12hrs.)

i) Solid-Phase Extraction and LC−MS analysis of Pyrrolizidine Alkaloids in Honeys.

ii) Comparative study of phytochemical screening, antioxidant and antimicrobial capacities of fresh and dry leaves crude plant extracts of *Datura metel* L.

Unit II – Biosynthesis of Metal Nanoparticles (12hrs.)

i) Green synthesis of silver nanoparticles using *Ixora coccinea* leaves extract.

ii) Ultrasmall Copper Nanoparticles Synthesized with a Plant Tea Reducing Agent.

Unit III – Characterization of Nanoparticles (12hrs.)

i) Phytosynthesis of silver nanoparticles using *Coccinia grandis* leaf extract and its application in the photocatalytic degradation

ii) A facile synthesis of high optical quality silver nanoparticles by ascorbic acid reduction in reverse micelles at room temperature.

Unit IV – Biological Applications of Nanoparticles (12hrs.)

i) The green synthesis, characterization and evaluation of the biological activities of silver nanoparticles synthesized from *Iresine herbstii* leaf aqueous extracts

ii) In vitro evaluation of antioxidant and anticancer potential of *Morinda pubescens* synthesized silver nanoparticles.

Unit V – Green catalytic activity of Nanoparticles (12hrs.)

i) Catalytic Reduction of 4-Nitrophenol using Biogenic Gold and Silver Nanoparticles Derived from *Breynia rhamnoides*.

ii) Catalytic degradation of organic dyes using biosynthesized silver nanoparticles.

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Paper-XII

Heterogeneous Catalysis

No. of Hrs – 4 / Week **Credits - 4**

Objectives

1. **To Learn about the prorous materials**
2. **To Understand the concept of metal doping and photocatalytic function of the material.**
3. **To study the catalytic and photocatalytic activity of the materials.**

Unit I

Zeolite-based photocatalysts - Zeolites and molecular sieves acting as hosts for photoactive guests - Electron donor photosensitisers - organic dye - electron acceptor photosensitisers - Zeolites encapsulating clusters of semiconductor oxides - Zeolites having photocatalytically active framework.

Efficient photocatalytic degradation of organics diluted in water and air using TiO2 designed with zeolites and mesoporous silica materials.

Unit II

Effect of metal-doping of TiO_2 nanoparticles on their photocatalytic activities toward removal of organic dyes.

Solar photocatalytic degradation of phenol using nanosized ZnO and α-Fe_2O_3.

Unit III

Network Structured SnO_2/ZnO Heterojunction Nanocatalyst with High Photocatalytic Activity.

Green synthesis of copper nanoparticles for the efficient removal (degradation) of dye from aqueous phase.

Unit IV

Visible Light Photodegradation of Phenol Using Nanoscale TiO_2 and ZnO Impregnated with Merbromin Dye: A Mechanistic Investigation.

Fe(III)/TiO_2-Montmorillonite Photocatalyst in Photo-Fenton-Like Degradation of Methylene Blue.

Unit V

TiO_2 nanoparticles immobilized on carbon nanotubes for enhanced visible-light photo-induced activity.

Preparation of a Titania/X-Zeolite/Porous Glass Composite Photocatalyst Using Hydrothermal and Drop Coating Processes.

References

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3. Egyptian Journal of Petroleum (**2014)** 23, 419–426
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