File Ref.No.24364/GA - IV - J2/2013/CU

UNIVERSITY OF CALICUT

Abstract

PG Diploma in Industrial Catalysis and Sustainable Chemistry-Syllabus-Approved - implemented w.e.f 2013 Admissions-Orders issued.

UNIVERSITY OF CALICUT

U.O.No. 5972/2013/CU Dated, Calicut University.P.O, 25.11.2013

Read:-1.Item no. 1 of the minutes of the meeting of the Board of Studies in Industrial Chemistry held on 10.09.2013.

2.Remarks of the Dean, Faculty of Science dated 15.11.2013.

3.Orders of the Vice Chancellor on 22-11-13 in the file of even no..

ORDER

The Board of Studies in its meeting held on 10.09.2013, resolved to approve the syllabus for PG Diploma in Industrial Catalysis and Sustainable Chemistry proposed by the St.Thomas College Trichur,and suggested that Industrial Training / Project Work for a duration of three months shall be included as part of the curriculum. as per paper read as (1).

Vide paper read as (2), the Dean Faculty of Science has approved the recommendations of the Board for implementation.

The Vice Chancellor, considering the exigency, excercising the powers of the Academic Council, has approved the item regarding the syllabus, with the suggestion of the Board, for implementation,.

Sanction has, therefore, been accorded for implementing the Syllabus of PG Diploma in Industrial Catalysis and Sustainable Chemistry, with Industrial Training / Project Work for a duration of three months as part of the curriculum, under the University with effect from 2013 admissions.

Orders are issued accordingly.

(The Syllabus is available in the Official website of the University:universityofcalicut.info)

Muhammed S
Deputy Registrar

To

Al the Institutions affiliated to/under the University of Calicut.

Forwarded / By Order

Section Officer

ST. THOMAS' COLLEGE, THRISSUR, KERALA

UNIVERSITY OF CALICUT

UGC SPONSORED INNOVATIVE PROGRAM

P G DIPLOMA IN INDUSTRIAL CATALYSIS AND SUSTAINABLE CHEMISTRY

(COURSE AND SYLLABUS)

SEMESTER I

Course code	Paper	Credit	Marks		Total marks
			Internal	External	
CHE 101	Physical Chemistry of Catalysis	4	40	60	100
CHE 102	Catalyst Preparative Methods	4	40	60	100
CHE 103	Modern Trends in Catalysis	4	40	60	100
CHE 104	Lab course-1	4	100	---	100
CHE 105	Lab course-2	4	100	---	100

SEMESTER II

Course code	Paper	Credit	Marks		Total marks
			Internal	External	
CHE 106	Catalysis – Industrial Applications	4	40	60	100
CHE 107	Catalysis and Sustainability	4	40	60	100
CHE 108	Research Methodology	4	40	60	100
CHE 109	Project and Viva	8	80	120	200

CHE – 101 PHYSICAL CHEMISTRY OF CATALYSIS
4 credits

60 hours

UNIT I

The solid liquid interface – surface area of solids – structure and chemical nature of solid surfaces – nature of the solid adsorbate complex – adsorption of gases and vapours on solids – comparison of surface area from various multilayer nodels - phase transformations in the multiplayer region – thermodynamics of adsorption. Physical adsorption on heterogeneous surfaces – rate of adsorption –chemisorption and catalysis – adsorption isotherms – kinetics of chemisorptions.

UNIT II

Chemical dynamics at surfaces – inelastic collision and trapping – the sticking coefficient – physisorbed molecules – molecule migration, desorption and transition to chemisorbed state – accommodation coefficients – energy exchange at surface – cube models. Precursor theory of chemisorption – sticking probability curves – their temperature dependence – example of N_2 on W. Desorption – analysis of desorption curves – kinetics of adsorption and desorption. The role of lattice imperfections in heterogeneous catalysis.

UNIT III

Catalyst selectivity – an empirical and kinetic method of estimating selectivity in consecutive reactions – kinetics of the selective formation of intermediate product in consecutive reactions – localized and mobile adsorption of the intermediate product – effect of pore size on catalyst selectivity – poly-functional catalysis –selectivity of poly-functional catalysis – thermodynamics of poly-step reactions.

UNIT IV

Determination of surface area and pore structure of catalysts – physical adsorption methods – mercury intrusion methods – chemisorption methods – X-ray methods – microscopic methods – radioactive isotope method – flow rate and diffusion methods – miscellaneous methods – comparison of methods. Adsorption from gas phase – hydrogen-deuterium exchange reactions applications of field emission microscopy (FEM); Scanning tunneling and atomic force microscopy (STM, AFM); Incident ion techniques – charge exchange between ions and surfaces – applications in ion scattering techniques – low energy ion scattering (LEIS) – application of LEIS in catalysis –model catalysts – single crystal studies. Surface crystallography- surface structure determination using low energy electron diffraction (LEED).

UNIT V

Principles and instrumentation of Gas Chromatography–Mass Spectrometry (GC-MS) – application in catalysis studies. Infrared spectroscopy - application of infrared spectroscopy to adsorption and catalysis. Raman spectroscopy – theory of Raman Effect – application of Raman spectroscopy to catalysis. Nuclear magnetic resonance spectroscopy – solid state NMR – basic principles and methods of solid state NMR. Electron spin resonance spectroscopy – features of ESR spectra – g value – shifts in g value – tensor properties of g and A parameter – origin of hyperfine interaction –

REFERENCE

1. A.W. Adamson & A.P. Gast, "Physical Chemistry of Surfaces", John Wiley and Sons, Canada, 1997.
2. R.H.P. Gasser, "An introduction to chemisorption and catalysis by metals", Oxford, 1985.
3. A. Clark, "Theory of adsorption and catalysis", Academic Press, New York, 1970.
4. D.K. Chakraborthy, "Adsorption and catalysis by solids", Wiley Eastern Ltd. 1990.
5. J.M. Thomas & W.J. Thomas, "Introduction to principles of heterogeneous catalysis", Academic Press, New York, 1967.
6. Viswanathan, S. Sivasanker, and A. V. Ramaswamy, Catalysis: Principles and Applications, Narosa Publishing House, New Delhi, 2002.
7. Bond, G. C Heterogeneous Catalysis: Principles and Application. Oxford Univ Press 1987.
8. R.B. Anderson, "Experimental methods in catalysis research", Vol 1-3, Academic press, New York, 1981.
9. W.M.A. Niessen, "Current Practice of Gas Chromatography – Mass Spectrometry", Marcel Dekker Inc, New York, 2001.
10. W.N. Delgass, G.L. Haller, R. Kellerman and J.H. Lunsford, "Spectroscopy in heterogeneous catalysis", Academic press, New York, 1979.
11. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 2, Wiley-VCH, Weinheim, 1997.
12. D.P. Woodruff and T.A. Delchar, "Modern techniques of surface science", Cambridge University press, 1990.
13. J.W. Niemantsverdriet, "Spectroscopy in Catalysis: an introduction", VCH, NY, 1995.
14. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 2 & 3, Wiley-VCH, Weinheim, 1997.
15. B.D. Cullity, Elements of X-ray Diffraction, Addison -Wesley, 1978.
16. Introduction to Photoelectron Spectroscopy (Chemical Analysis Vol. 67) P. K. Ghosh, Wiley, Interscience, 1983.
17. Spectroscopy in Catalysis J. W. Niemantsverdriet, VCH Publishers, 1995.
18. D.Briggs and M.P.Seah (Editors) Practical Surface Analysis - Auger and X-ray Photoelectron Spectroscopy, , Wiley Interscience, 1990 (2nd ed.).
19. Introduction to Photoelectron Spectroscopy (Chemical Analysis Vol. 67) P. K. Ghosh, Wiley Interscience, 1983.

CHE- 102 CATALYST PREPARATIVE METHODS
4 credits

60 hours

UNIT I

General preparative methods – precipitation and coprecipitation – sol gel process – flame hydrolysis – supported catalysts from CVD and related techniques – Dispersed metal catalysts; support materials; preparation and structure of supports; surface properties – preparation of catalysts – introduction of precursor compound – interaction of metal compound with substrate surface – metal distribution within catalyst pellets.

Catalyst manufacture – equipment – scope and goals – catalysts prepared by precipitation – solution and slurry transfer – filtration – drying: containers, trays and other drying auxiliaries;

calcining; rewashing and ion exchange; pulverization, pilling and extrusion; crushing and screening to produce granules; coating (not impregnation); impregnation to orient the coating material to the support – anchor coating or wash coating.

UNIT II

Bulk catalysts and supports – fused catalysts – Skeletal metal catalysts – Metallic glasses – Heteropoly compounds – Solid superacids – Carbons – structural chemistry of carbon – overview – basic structures – loosely defined structures – formation of carbon materials: general pathways, mechanistic aspects – catalytic formation of carbon from molecules – carbon on noble metal catalysts – carbon formation in zeolites – graphitization of carbon – reaction of oxygen with carbon – surface chemistry of carbon – non-oxygen hetero elements on carbon surfaces – surface oxygen groups – carbon as catalyst support – carbon as catalyst.

UNIT III

Synthesis of aluminosilicate zeolites and related silica based materials – structure, composition, nomenclature – zeolite synthesis, mechanism and chemistry – experimental part – experimental factors – review of zeolites obtained from various reaction systems – synthesis of some selected important zeolites – metals supported on zeolites – reduction of metal ions in zeolite – dealumination of zeolites; Shape selective catalysis in zeolites.

Pillared clays – properties of pillared clays – recent advances in the synthesis and catalytic applications of pillared clays –the use of coordination and organometallic compounds as pillaring agents – the use of polymers and surfactants in pillaring process; Mesoporous materials – zeolites containing mesopores –synthesis of silica molecular sieve materials – catalytic properties of mesoporous materials with long-range crystallinity.

UNIT IV

Design of industrial catalysts; design procedure; the overall design of catalysts – overall development of an industrial catalyst – scientific basis of design – the idea – preliminary checking – the description of the idea – theoretical design: primary components of the catalyst - components of a catalyst – selection of the preferred form of a catalyst – the overall design; alloy catalysts – metal cluster catalysts – metal oxide solid solutions – specific examples of oxide solid solution catalysts applied to design; choice of support materials. Specific examples of catalyst design; design of a catalyst for conversion of olefins to aromatics – description of the idea – design of primary constituents – experimental testing – design of secondary components; design of a catalyst for selective hydrogenation of acetylene in presence of ethylene – description of the idea – co-ordination and geometric considerations and design – catalysis by metals.

UNIT V

Deactivation of catalysts – classification of catalyst deactivation processes; general aspects of catalyst deactivation – poisoning of catalysts – poisoning of metallic catalysts – poisoning of non metallic catalysts – poisoning of bifunctional catalysts – coke formation on catalysts – metal deposition on catalysts – sintering of catalysts; diffusion and deactivation of catalysts – analogy between selectivity and deactivation mechanisms.

Regeneration of deactivated catalysts – feasibility of regeneration – description of coke deposit and kinetics of regeneration – regeneration of coked catalyst pellets – regeneration of fixed beds containing coked catalysts; Technological economics; Catalytic processes in an integrated system – effect of catalyst on plant equipment – catalyst life – effect of improvement in catalyst performance on process and economics – prospects for new catalytic process.

REFERENCE

1. G. Ertl, H. Knozinger and J. Weitkamp (eds), "Preparation of Solid Catalysts", Wiley-VCH, Verlag, 1999.
2. J.R. Anderson and M. Boudart (Eds), "Catalysis, Science and Technology", Vol 6, Springer-Verlag, Berlin Heildberg, 1984.
3. J. Weitkamp and L. Puppe (eds), "Catalysis and zeolites – fundamentals and applications", Springer-Verlag Berlin Heidelberg 1999.
4. A. Corma, Chemical Reviews, 97 (1997) 2373-2419.
5. S. van Donk, A.H. Janssen, J.H. Bitter & K.P. deJong, Catalysis Reviews, 45 (2003) 297-319.
6. A. Gil, L.M. Gandia & M.A. Vincente, Catalysis Reviews Science and Engineering, 42 (2000) 145-212.
7. B.F. Sels, D.E. De Vos & P.A. Jacobs, Catalysis Reviews, 43 (2001) 443-488.
8. M. Hartmann & L. Kevan, Chemical Reviews, 99 (1999) 635-663.
9. A.B. Stiles and T.A. Koch, "Catalyst manufacture", Marcel Dekker Inc., NY, 1995.
10. R. Hughes, "Deactivation of catalysts", Academic press, London, 1984.
11. R. Pearce and W.R. Patterson, "Catalysis and chemical processes", Academic press, Leonard Hill, London, 1981.
12. C.A. Heaton (ed), "An Introduction to Industrial Chemistry", Leonard Hill, London, 1984.
13. D.L. Trimm, "Design of industrial catalysts", Elsevier scientific, NY, 1980.

CHE – 103 MODERN TRENDS IN CATALYSIS

4 credits

60 hours

UNIT I Phase Transfer Catalysis: Basic concepts in phase transfer catalysis –use of quaternary salts – macrocyclic and macrobicyclic ligands – PEG's and related compounds –use of dual phase transfer catalyst or co-catalyst in phase transfer systems –separation and recovery of phase transfer catalysts. Insoluble phase transfer catalysts – PTC catalysts bound to resins – phase transfer catalysts bound to inorganic solid supports – phase transfer catalysts contained in separate liquid phase (third liquid phase catalyst); Variables in reactor design for application of PTC.PTC displacement reactions with simple anions –behaviour of various anions in PTC displacement reactions Phase transfer catalyzed oxidations –PTC reductions –PTC: Chiral phase transfer catalyzed formation of C-C bonds

UNIT II Electrocatalysis: The science of electrocatalysis on bimetallic surfaces, fundamental aspects of vacuum and electrocatalytic reactions of methanol and formic acid on Pt surfaces – UHV models of electrocatalysis – electrocatalytic mechanism and kinetics – poisoning – reaction modifiers. Electrocatalytic hydrogenation of organic compounds – Recent advances in kinetics of oxygen reduction – gas phase studies of oxygen chemisorptions. Studying electrocatalytic oxidations of small organic molecules with in-situ IR spectroscopy – principles and methods of in-situ IR spectroscopy – in-situ time resolved IR spectroscopic studies of the kinetics of

electrocatalytic oxidation of small organic molecules. Unified model of electron and ion transfer reactions at metal electrodes – extended Anderson-Newns model – electro-reductions of anions – double layer effects at single crystal electrodes – ion transfer reactions – electron transfer to adsorbed reactants – electron and proton transfer at self assembled monolayer.

UNIT III Biocatalysis: Enzymes – an introduction to enzymes – enzymes as proteins – classification and nomenclature of enzymes – structure of enzymes – how enzymes work – effect on reaction rate – thermodynamic definitions – catalytic power and specificity of enzymes – optimization of weak interactions between enzyme and substrate in the transition state – binding energy, reaction specificity and catalysis – kinetic parameters used to compare enzyme activities. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes. Lewis acid properties of Zn and its development to phosphotriester detoxifying agents – vanadium haloperoxidases – Mo and W enzymes – catalysis by nitrogenases and synthetic analogs – biological Fe-S clusters with catalytic activity. Catalysis by Ni in biological systems – oxygen activation at non-heme iron centers – dioxygen activation at heme centers in enzymes and synthetic analogs. Biochemical reaction systems – enzyme fermentation – Microbial fermentation – mixed flow fermentors. Biological and biomimetic catalysis. The concept of organo catalysis. Immobilized biocatalysts – definition and classification of immobilized biocatalysts – immobilization of coenzymes.

UNIT IV Nano catalysis: General definition - nanochemistry basics - distinction between molecules, nanoparticles and bulk materials. Physico-chemical considerations (geometric and electronic structures, reactivity) of nanomaterials. Size dependent properties. Interfacial, colloidal, surfactant and supramolecular chemistry. Preparation (sonochemical, precipitation, sol-gel, chemical-vapour deposition, gas-phase condensation, template-mediated, electro-deposition, solvo-thermal, etc.) and fabrication (zero-, one- and twodimensional nanostructures) of nanomaterials. Characterization of nanomaterials by diffraction, spectroscopy and microscopy techniques. Nanomaterials including molecular sieves, dendrimers, inorganic-organic hybrids. Potential relevance of organic and inorganic nanostructures for advanced material science, organic synthesis, catalysis, and adsorption/separation processes. Risk discussion and future perspectives.

UNIT V Polymer supported catalysis: Preparation of functionalized polymers –polystyrene, biopolymers and inorganic supports functionalisation - condensation polymers functionalisation – functionalisation by grafting. Organic reactions using polymer supported catalysts – polymer supported multistep organic synthesis - industrial applications. Hydrogenation processes catalyzed by metal containing polymers – Oxidation reactions catalyzed by immobilized metal complexes – polymeric metalloporphyrin catalyzed olefin oxidation – catalase type activity – metal polymer catalyzed olefin epoxidation by alkyl hydroperoxides – Activation of small stable molecules and stimulation of catalytic reactions through participation of immobilized metal complexes –water gas shift reaction – Photochemical decomposition of water.

REFERENCE

1. A. Akelah & A Moet, "Functionalized polymers and their applications", Chapman and Hall, 1990.
2. D.C. Sherrington & P. Hodge, "Synthesis and separations using functional polymers", John Wiley and Sons, 1988.

3. A.D. Pomogailo, "Catalysis by polymer-immobilized metal complexes", Gordon & Breach Science Publishers, Amsterdam, 1998.
4. C.M. Starks, C.L. Liotta and M. Halpern, "Phase Transfer Catalysis – fundamentals, applications and industrial perspectives", Chapman & Hall, New York, 1994.
5. Y. Sasson and R. Neumann (eds), "Handbook of Phase Transfer Catalysis", Chapman & Hall, Great Britan, 1997.
6. J. Lipkowski and P.N. Ross, "Electrocatalysis", Wiley VCH, Canada, 1998.
7. J. O'M. Bockris and S.U.M. Khan, "Surface Electrochemistry", Plenum press, New York, 1993.
8. J. O'M. Bockris, A.K.N. Reddy and M. G-. Aldeco, "Modern Electrochemistry – fundamentals of electrodics", IInd edition, Kluwer academic/Plenum press, New York, 2000.
9. A.L. Lehninger, "Principles of Biochemistry", Worth Publishers, USA, 1987.
10. W. Hartmeier, "Immobilized Biocatalysts: an introduction", Springer-Verlag, Berlin Heidelberg, 1986.
11. J. Reedijk and E. Bouwman, "Bioinorganic Catalysis", Marcel Dekker Inc. New York, 1999.

CHE 104 LAB COURSE -1

4 credits

4 hours / week

Students are expected to do at least six (6) experiments out of the following type(s)

1. Preparation of supports for catalysts – alumina, silica, zeolites, titania.
2. Comparison of different preparation techniques – precipitation, precipitation from homogeneous solution, polymer pyrrolysis, template synthesis, sol-gel method etc.
3. Surface area determination of catalysts.
4. Spectroscopic measurements (UV-VIS and FT-IR)
5. Shaping of support materials to extrudates and spheres.
6. Preparation of dispersed metal oxide catalysts – co precipitation, impregnation techniques.
7. Conversion of active phase into metal form – reduction.
8. Measurement of acidity of catalysts – Temperature Programmed Desorption of ammonia, adsorbed ammonia IR spectra.
9. Characterization of surface functional groups using IR spectroscopy.
10. Synthesis of polymer supports and its functionalization.

References:

1.Anderson Robert, Experimental methods in catalytic research, New York, 1968, 498 .pp, hard cover,

2. Anderson Robert and Peter T.Dawson, Experimental methods in catalytic research, Academic Press, N.Y.,1976.

CHE 105 LAB COURSE -2

4 credits

4 hours / week

Students are expected to do at least six (6) experiments out of the following type(s)

1. Synthesis of trasitionmetal precursors and their transformations
2. Synthesis and characterization of some transition metal complex catalysts using conductance, magnetic susceptibility and IR.
3. Application of some transition metal complex in amination and coupling reactions and product analysis by GCMS.
4. Synthesis and electrochemical studies on transition metal complexes.
5. Oxidation of *p*-xylene to tere-phthalic acid using $Co(II)Br_2$.
6. Transfer hydrogenation using organometallics and product studies using GCMS.
7. Metalloporphyrin synthesis and its use in the activation small molecules – UV studies.
8. Fabrication of reactors and activity studies for hydrogenation reactions using pulsed micro-catalytic reactors and continuous flow reactors.
9. Activity studies for F C alkylation and acylation reactions and analysis by GCMS.
10. Synthesis of ionic liquids.

References:

1.Anderson Robert, Experimental methods in catalytic research, New York, 1968, 498 .pp, hard cover,

2. Anderson Robert and Peter T.Dawson, Experimental methods in catalytic research, Academic Press, N.Y.,1976.

CHE 106 CATALYSIS - INDUSTRIAL APPLICATIONS

4 credits

60 hours

UNIT I

Homogeneous reactions. Importance of homogeneous catalysis in the synthesis of high value chemicals. Organo-metallics and importance of ligands. Ligand cone angles – steric effects– catalytic cycles. Turnover number and frequency. Kinetics of homogeneous reactions – concentration dependent term – temperature dependent term – searching for a mechanism – predictability of reaction rate from theory – Reactions in ideal reactors. Interpretation of batch reactor data – constant volume and varying volume batch reactor – temperature and reaction rate.

UNIT II

Hydrogenation reactions- Reversible cis-dihydrido catalysts- asymmetric hydrogenation- alkene isomerisation, hydrosilylation and hydroboration reaction- Reactions of Co and hydrogen- watergas shift reaction- Fischer –Tropsch reaction- hydroformylation of unsaturated compounds

carbonylation reactions- Oxo synthesis – production of acetic acid by carbonylation of methanol – selective ethylene oxidation by the Wacker process – oxidation of cyclohexane - Monsanto L-Dopa process, epoxidation of propene,

UNIT III

Oligomerization of ethylene (SHOP); Cluster compounds as homogeneous catalysts and catalyst precursors – classification of catalyst precursors based on structure. homogeneous and heterogeneous Zeigler-Natta catalysts – supported metal complex catalysts – Phillips process for ethylene polymerization; Late-metal catalysts for ethylene homo and copolymerization – effect of nature of metallocene complexes of group IV metals on their performance in catalytic ethylene and propylene polymerization – stereocontrol by metallocene catalysts. carbocationic alkene polymerizations initiated by organo transition metal complexes. Grubbs catalyst in polymerization.

UNIT IV

Polymer bound transition metal complex catalysts – synthesis of supports and catalysts – characterization by physical methods – catalysis – stability of polymer supported catalysts – comparison of polymers with inorganic catalyst supports; Specific features of catalysis by immobilized metal complexes – ligand exchange in metal-polymeric systems – characteristics of electron-transfer reactions – macromolecular effects – main factors regulating activity – effects of cluster formation and cooperative stabilization – outlook for polyfunctional catalysis – technological aspects.

UNIT V

Zeolite entrapped metal complexes – synthesis – flexible ligand method – ship in a bottle method – zeolite synthesis method – characterization – stability analysis – oxygen adsorption – cyclovoltametry – catalysis by zeolite entrapped transition metal complexes – ordered mesoporous and microporous molecular sieves functionalized with transition metal complexes as catalysts for selective organic transformations – propene polymerization with silica supported metallocene/MAO catalysts.

REFERENCE

1. F.A. Cotton, G. Wilkinson, C.A. Murillo & M. Bochmann, "Advanced inorganic chemistry", VI edition, John Wiley and sons, Singapore, 1999.
2. J.E. Huheey, "Inorganic chemistry: principles of structure and reactivity", Harper and Row publishers, Singapore.
3. J. Hagen, "Industrial catalysis: A practical approach", Wiley VCH, Weinheim, Germany, 1999.
4. D.C. Sherrington & P. Hodge, "Synthesis and separations using functional polymers", John Wiley and Sons, 1988.
5. A.D. Pomogailo, "Catalysis by polymer-immobilized metal complexes", Gordon & Breach Science Publishers, Amsterdam, 1998.
6. G. Ertl, H. Knozinger and J. Weitkamp, "Handbook of Heterogeneous Catalysis" Vol 3 and 5, Wiley-VCH, Weinheim, 1997.
7. G.W.Parshall and S.D.Ittel, Homogensous Catalysis, The applications and chemistry of catalysis by soluble Transition Metal Complexes, Wiley, New York, 1992.

8. B.Cornils and W.A.Herrmann, Applied Homogeneous catalysis with Organometallic Compounds, Vol 1 and 2, Weinheim, New York, 1996.
9. S.Bhaduri and D.Mukesh, Homogeneous Catalysis, Mechanism and Industrial Applications, Wiley, New York, 2000.
10. P.W.N.M.Van Leeuwen, Homogeneous Catalysis: Understanding the art, Kluwer, Academic Publishers, 2003.

CHE – 107 CATALYSIS AND SUSTAINABILITY

4 credits **60 hours**

UNIT I

Thermodynamics and relation to internal energy, Light and molecules: Photon field and Excited state, quantum yield, Kinetic Rate equations for photocatalysis: parallel, series, reactions, intensity, turnover rate. Photoprocesses at metals, oxides and semiconductors: concepts, discoveries and applications, Sensitization of photocatalysts and photosplitting of water.

UNIT II

Advances in design, preparation and characterization of photocatalysts: oxides, chalcogenides, semiconductors, layered materials, porous materials, artificial photosynthesis. Photocatalysis and the environment: water purification, organic degradation by photocatalysts, self cleaning photocatalysts, airborne pollutant degradation, reactors for photocatalysis. Photo cleavable protecting groups in organic synthesis. Photoelectrochemistry : concepts, discoveries and applications, storage and synthetic cells, energy generation, cell design, diagnosis and characterization of photoprocesses at electrodes.

UNIT III

Primary and secondary pollution; environmental damage, causes and remedies; Green house effects, ozone hole and causes for these; purification of exhaust gases from different sources: auto-exhaust catalysts (petrol vehicles); reactions involved, catalysts and their preparation, three-way catalysts, catalysts for diesel vehicles - NOx suppression methods, lean NOx trap, decomposition of NOx, selective catalytic reduction; deactivation of autoexhaust catalysts; purification of emissions from stationary units – catalysts and applications; catalytic combustion;VOC removal; ozone decomposition; photocatalysis in effluent treatment.

UNIT IV

Carbon dioxide and carbohydrates as feed stocks. Transformation of carbon dioxide and carbohydrates into useful products. Renewable energy sources. Recycling.

UNIT V

Principles of green chemistry: selectivity in catalysis; solid catalysts for organic reactions, solid acids and bases as catalysts, selective oxidation reactions; hydrogenation – dehydrogenation, catalytic carbon – carbon bond formation; catalysis in novel reaction media; cascade catalysis; renewable raw materials; examples of green process innovations: caprolactam, vanillin, adipic acid, phenol, polycarbonate; enantioselective catalysis; clean fuels.

REFERENCE

1. Photo-catalytic Reaction Engineering, Hugo De Lasa, Benito Serrano and Miguel Salaices, Springer, NewYork, NY, 2005.

2. Photo-catalysis: Science and Technology, Edited by Masao Kaneko and Ichiro Okura, Springer, NewYork, NY, 2003.

3. Photocatalysis: Fundamentals and Applications, Nick Serpone and Ezio Pelizzetti, Wiley, NewYork, NY, 1989.

4. Electrochemical Methods, Fundamentals and Applications, 2nd Edition, Allen J. Bard and Larry R. Faulkner, Wiley, NewYork, NY, 2001.

5. Semiconductor Electrodes and Photoelectrochemistry, Volume 6, Encyclopedia of Electrochemistry, Edited by Stuart Licht and Maheshwar Sharon, Wiley, NewYork, NY, 2002.

6. Semiconductor Photoelectrochemistry, Samir J. Anz, Arnel M. Fajardo, William J. Royea and Nathan S. Lewis, p 605-636, Wiley, NewYork, NY, 2003.

CHE-108 RESEARCH METHODOLOGY IN CHEMISTRY

4 credits

60 hours

UNIT I

Research methodology and data analysis: Research processes – scientific research, formation of the topic, hypothesis, conceptual definition operational definition, gathering of data, analysis of data, revising of hypothesis, Conclusion. Literature survey – Journal

Books and e-resources. Presentation and publication of research output. Errors in chemical analysis, classification errors, determination of accuracy of methods, improving accuracy of analysis, significant figures, mean, standard deviation, comparison of results: "t" test, "f" test and "chi" square test, least squares analysis, weighted least squares analysis, regression coefficient, rejection of results, presentation of data.

UNIT II

Applications of Computers in Chemistry: of development of computers, mainframe, mini micro's and supercomputer system. Personal computers. General awareness of computer hardware, CPU, input and output devices, memory, other peripheral devices, auxiliary storage devices.

Basic knowledge of computer systems, soft wares-system soft wares and application soft wares Programming languages: Machine language, assembly language and high level languages. Interpreter and compiler. Flow charts and Algorithms. General awareness operating systems: Disk operating system, windows, Macintosh, Linux. General awareness of soft ware packages and other scientific application packages. Application and uses of common soft wares in chemistry, Origin, Chemsketch, Chemdraw. Basic ideas on the use of internet in chemistry education.

UNIT III

Chromatographic techniques: Gas chromatography: Theory of chromatography, column efficiency and column equation, sample injection, sampling system for capillary columns and packed columns, detectors, gas

flow control system, high resolution gas chromatography/mass spectroscopy. HPLC: principles of high performance liquid chromatography, the liquid chromatograph, the requirements of solvent pumping and different pumping systems, gradient elution, isocratic elution, sampling, detectors for liquid chromatography, the mobile phase in HPLC, solvent degassing, column technology, column selection, quantitative analysis by HPLC.

UNIT IV

Analytical techniques for chemical research: Optical methods of analysis, basic principles of uv-visible, AAS, AES, flourometric and phosphorometric methods. Electroanalytic methods-Principles and applications of polarography, amperometry, coulometry and cyclicvoltametry.

Thermal methods of analysis- Principles and important applications of thermogravimetry (TG)- differential thermal analysis (DTA), differential scanning calorimetry (DSC), dilatometry (DIL) and dynamic mechanical analysis (DMA).

UNIT V

Physical methods for structure elucidation: An integrated problem solving approach to the elucidation of structures of organic compound based on UV, IR, NMR (^{1}H and ^{13}C) and Mass spectral techniques. Modern NMR experiments: NOE, APT,DEPT,HOMCOR (^{1}H -^{1}H) and HETEROCOSY (1H-13C). Use of electronic, IR, NMR, (1H,13C, 19F, 31P), Mossbauer and ESR in the structure elucidation of inorganic and coordination compounds.

REFERENCE

1. Paul D Leedy, Jeanne E Ormrod and Jeanne Ellis Ormord, Practical Research :Planning and Design, Prentice Hall, 2004.
2. Robert V Smith, Graduate Research: A Guide for students in the Sciences, University of Washington Press,1998.
3. Peter C Jurs, Computer Software Application in Chemistry, 2nd Ed., John Wiley & Sons, new York, 1996.
4. K V Raman, Computers in Chemistry, Tata McGraw Hill, 1993.
5. Ramesh Kumari Computers and their applications Chemistry, 2nd Edition, Alpha Science Intl Ltd, 2005..
6. Cropper William H, Mathematical Computer Programs for Physical Chemistry, Springer, 1998.
7. Stephen Wilson, Chemistry by Computer: An Overview of the Applications of Computers in Chemistry, Plenum Pub Corp, 1986t.
8. Peter C Jurs, Computer Soft ware Applications in Chemistry, 2nd Ed., John Wiley & sons new York, 1996.
9. Hobart H Willard, Lynne L Merritt, Jr., Jonn A Dean, Frank A Settle, Jr (Ed.), Instrumental Methods of Analysis, 7th Ed., WADSWORTH publishing company, 1988.
10. DA Skoog and M West, Fundamentals of Analytical Chemistry, Saunders Golden Sunburst Series.
11. WW Wendlandt, Thermal Methods of Analysis, Interscience, New York, 1964.
12. PJ Haines, Thermal Methods of Analysis: Principles, Applications and problems, Blackie Academic and Professional, New York, 1995.
13. GWH Hohne, WH Hemmin ger and HJ Flammersheen, Differential Scanning Calorimetry, 2nd Edition, Springer.
14. RM Silverstein, CG Bassler and TC Morril, Spectroscopic Identification of Organic Compounds, 4th Edition, John Wiley & Sons, New York, 1981.
15. Donald L Pavia, Gary M Lampman and George S Kriz, Introduction to Spectroscopy, 3rd Edition, Saunders Golden Sunburst Series.