M.Tech. Course in Catalysis Technology

CURRICULUM AND COURSE CONTENTS

INDIAN INSTITUTE OF TECHNOLOGY MADRAS
CHENNAI 600 036

M.Tech. (Catalysis Technology)

I SEMESTER

Course ID	Course Name	L	T	P	C
CA501	Fundamentals of Adsorption and Catalysis	3	0	0	3
CA502	Solids and Surfaces	3	0	0	3
CH501	Chemical Reactor Theory	3	1	0	4
CH502	Experimental and Analytical Methods in Chemical Engineering	3	0	0	3
CA	Elective 1	3	0	0	3
CA	Elective 2	3	0	0	3
	Total Credits	**18**	**1**	**0**	**19**

Semester I - Electives

Course ID	Course Name	L	T	P	C
CA511	Preparation and Properties of Catalysts	3	0	0	3
CA512	Homogeneous Catalysis	3	0	0	3
CA513	BioCatalysis	3	0	0	3
CA514	Computational Methods in Catalysis	3	0	0	3

II SEMESTER

Course ID	Course Name	L	T	P	C
CA503	Experimental Methods in Catalysis	3	0	0	3
CA504	Introduction to Surface Analysis	3	0	0	3
CH503	Transport Phenomena	3	1	0	4
CA505	Catalyst Preparation and Characterization Laboratory	0	0	3	1
CA	Elective 3	3	0	0	3
CA	Elective 4	3	0	0	3
	Total Credits	**15**	**1**	**3**	**17**

Semester II - Electives

Course ID	Course Name	L	T	P	C
CA515	Catalysis in Petroleum Technology	3	0	0	3
CA516	Catalysis in Production of Chemicals	3	0	0	3
CA517	Nano-materials in Catalysis	3	0	0	3
CH516	Chemical and Catalytic Reaction Engineering	3	0	0	3

III SEMESTER

Course ID	Course Name	L	T	P	C
CA651	Project (Stage I)	-	-	-	6*
CA652	Seminar I	-	-	-	1
CA	Elective 5	3	0	0	3
CA	Elective 6	3	0	0	3
	Total Credits	**6**	**0**	**0**	**7**

**Credits to be assigned and added to the IV semester.*

Semester III - Electives

Course ID	Course Name	L	T	P	C
CA611	Catalysis in Green Chemistry and Environment	3	0	0	3
CA612	Photocatalysis	3	0	0	3
CH604	Chemical Reactor Design for Process Plants	3	0	0	3
CH612	Particle Characterization	3	0	0	3
CH615	Multiphase Reactors	3	0	0	3
CY672	Chemical and Electrochemical Energy Systems	3	0	0	3
CY 676	Principles of Surface Chemistry	3	0	0	3

IV SEMESTER

Course ID	Course Name	L	T	P	C
CA651	Project (Stage II)	-	-	-	20*
CA653	Seminar II	-	-	-	1
	Total Credits	**-**	**-**	**-**	**21**

- **Inclusive of 6 Credits from III semester.**

Total credits = 19 + 17+7 +21 = 64

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Fundamentals of adsorption and catalysis</td><td>Course No.</td><td colspan="4">CA 501</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M Tech Catalysis Technology</td><td>Status</td><td colspan="2">Core</td><td colspan="2"></td></tr>
<tr><td>Faculty</td><td>Prof. B Viswanathan
Prof. AV Ramaswamy
Prof . S Sivasanker</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">JULY 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives: To deal with the adsorption process which is fundamental to catalysis both theory and experimental evaluation

   To outline the utility of adsorption process for evaluating the texture and also surface properties of catalysts.

2. Course Contents: Physical and Chemical adsorption – adsorption isotherms: evaluation of the texture of solids: chemisorption bond, chemisorption on metals and oxides. Catalysis: concepts – evolution, model catalytic reactions for elucidation; H_2¬D_2 exchange, ethylene hydrogenation, CO oxidation and hydrocarbon reactions.

Review of catalysis: Concepts like multiplet theory, ensembles, geometric factor; local field effects; coupled interactions; structure sensitivity and structure insensitivity; demanding reactions site structure; molecularity; remote control and auto-remote; bi- and multi-functionality; forward and back spillover; bifurcation theory; bi-and multi layers; bond order conservation; electrochemical promotion; kinetic coupling; linear free energy relationships; metal-support interactions; pore efficiency and effectiveness; self organization; sorbate-sorbate interactions; structure breaking and directing; structure-reactivity relationships; templating; poisoning, promotion and deactivation; selectivity; catalytic process engineering: examples and case histories; environmental and green chemical concepts.

3. Text Books and References:

1. John Meurig Thomas and W. John Thomas, Principles and Practice of Heterogeneous Catalysis (Paperback), Acdemic press
2. Michael Bowker, The Basis and Applications of Heterogeneous Catalysis (Oxford Chemistry Primers, 53) (Paperback).
3. A. W. Adamson ,Physical Chemistry of Surfaces , , Wiley Intersciences, 1990 (5th edition) 1990.
4. Bond, G C , Heterogeneous Catalysis: Principles and Application. Oxford University Press 1987.
5. D.K. Chakrabarty and B. Viswanathan, Hetergogeneous Catalysis, 2008 New Age Int. Publ.
6. B. Viswanathan, S. Sivasanker, and A. V. Ramaswamy, Catalysis: Principles and Applications, (Hardcover - 9 April 2002), Narosa Publishing House, New Delhi

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Solids and Surfaces</td><td>Course No.</td><td colspan="4">CA902</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2">Core</td><td colspan="2"></td></tr>
<tr><td>Faculty</td><td>Prof. P Selvam
Prof. B Viswanathan</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">JULY 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:
   To consider the structures of solids
   The study of the structure of solids
   Diffraction methods

2. Course Contents:
   Structure of solids. Lattice energy. Diffusion in solids. Crystal defects, Non-stoichiometry and Solid solutions. Solid state transformations and reactions. Crystal Chemistry, Property and Application of Materials. Surface structure, notation, clean and stepped surfaces; reconstruction, structure of adsorbate layers, molecular chemisorption, surface energy, Bonding in solids. X-ray diffraction: indexing of reflections, determination of lattice type, lattice extinctions, application and interpretation of powder X-ray diffraction data. Neutron and electron diffraction.

3. Text Books and References:

   1.H. V. Keer, Principles of the Solid State, New Age International, 1996.
   2.L. Smart and E. More, Solid State Chemistry, Chapman & Hall, 1993.
   3.C. Kittel, Introduction to Solid State Physics, Wiley, 1991.
   4.A.W. Adamson, Physical Chemistry of Surfaces, Wiley, 1990.
   5.A. R. West, Solid State Chemistry and Its Applications, Wiley, 1989.
   6.A. Zangwill, Physics at Surfaces, Oxford University Press, 1988.
   7.B.D. Cullity, Elements of X-ray Diffraction, Addison -Wesley, 1978.
   8.L.V. Azaroff, Introduction to Solids, Tata McGraw-Hill, 1977.

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Experimental methods in Catalysis</td><td>Course No.</td><td colspan="4">CA 503</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">CHEMICAL ENGINEETING (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M Tech Catalysis Technology</td><td>Status</td><td colspan="2">Core</td><td colspan="2"></td></tr>
<tr><td>Faculty</td><td>Prof. B. Viswanathan
Prof A V Ramaswamy
Prof S Sivasanker</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">JULY 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

The main objective is to give a foundation in various experimental methods of studying catalysts and catalytic processes.

2. Course Contents:

Physico-chemical characterization of catalysts using a variety of technique:
Adsorption measurements, specific surface area, metal surface area, pore volume, pore size distribution, Different methods, t-plots.
Structure characterization techniques, ESR, NMR for the study of solid catalysts
Magnetic properties and measurements
Electrical properties and measurements as a function of adsorption and catalysis.

3. Text Books and References:

1.R.B.Anderson Experimental methods in Catalysis Vol 1-3 Academic Press, New York, 1976.
2. S.Greg and K Sing, Adsorption, specific surface and Porosity
3. H.Van Bekkum et al (Editors) Introduction to zeolite Science and Practice, Elsevier, Amsterdam, 2001.

DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS
(NCCR)
Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Introduction to Surface analysis</td><td>Course No.</td><td colspan="4">CA 504</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M. Tech
Catalysis Technology</td><td>Status</td><td colspan="3">Core</td><td></td></tr>
<tr><td>Faculty</td><td>Prof. B Viswanathan
Prof A V Ramaswamy
Prof P Selvam
Prof G Renga Rao (to be invited)</td><td>Type</td><td colspan="3">New</td><td></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">JULY 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:
   Surface analysis has undergone much change in the last three decades and to familiarize the methods available.

2. Course Contents:
   Classification of techniques on the basis of input and output probes.
   Thermal in neutral out techniques, TPX methods qualitative and quantitative aspects of TPX techniques. Temperature-programmed technique: pulse adsorption; temperature-programmed reduction and desorption; surface acidity estimation
   Photon in techniques – Spectroscopic methods in catalyst characterization: UV-Vis and FT-IR spectral analysis of catalysts and surfaces. **Photoelectric effect**: basic principles of electron spectroscopy, classification of various spectroscopies.
   Photoelectron spectroscopy: XPS and UPS) experimental methods-electron energy analysis-photon sources -- angular dependence-cross section and its determination-valence and core photoemission - Koopmans' theorem-quantum chemical methods-final state effects
   Electron energy loss spectroscopy: Franck and Hertz experiment -- instrumentation -selection rules-theory - studies on molecules - surface states - high resolution spectroscopy - adsorption and catalysis -applications.
   Auger electron spectroscopy: introduction - instrumentation - classification of various transitions - applications
   Related techniques: inverse photoemission - spin resolved photoemission - recent advances in instrumentation-brighter photon sources.
   Electron in techniques – AES and EELS techniques, EIS
   Ion in techniques ISS and other ion sputtering techniques

3. Text Books and References:

1. Introduction to Photoelectron Spectroscopy (Chemical Analysis Vol. 67) P. K. Ghosh, Wiley Interscience, 1983.
2. Spectroscopy in Catalysis J. W. Niemantsverdriet, VCH Publishers, 1995.
3. J.T.Grant, Auger Electron Spectroscopy - AVS Training Course Book University of Dayton, 1994
4. D.Briggs and M.P.Seah (Editors) Practical Surface Analysis - Auger and X-ray Photoelectron Spectroscopy, , Wiley Interscience, 1990 (2nd ed.)
5. K. Seigbahn et.al., ESCA applied to Free Molecules", North Holland Publishing Company", 1969.
6. A. D. Baker and C. R. Brundle, Eds, "Electron Spectroscopy" Vol. 1 - 4 Academic Press, 1978.
7. H. Ibach and D. L. Mills, "Electron Loss Spectroscopy and Surface Vibrations", Academic Press, 1982
8. H. Ibach, "Electron Energy Loss Spectroscopy", Springer Verlag, 1992.
9. J. W. Rabalais, "Principles of Ultraviolet Photoelectron Spectroscopy". Wiley- Interscience, 1975 .
10. J. Berkowiz, "Principles of Ultraviolet Photoelectron Spectroscopy". Academic Press, 1975
11. P. Karsky and M. Urband, "Ab-Initio MO Calculations" Lecture Notes in Chemistry , Springer Verlag, 1980.
12. G.A.Somorjai, Introduction to Surface Chemistry and Catalysis, 1994.

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Catalyst preparation and characterization Lab</td><td>Course No.</td><td colspan="4">CA 505</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>0</td><td>0</td><td>3</td><td>1</td></tr>
<tr><td>Offered for</td><td>M Tech Catalysis Technology</td><td>Status</td><td colspan="2">Core</td><td colspan="2"></td></tr>
<tr><td>Faculty</td><td>Prof P Selvam
Prof S Sivasanker</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">July 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

To give hands on experience some basic measurements in catalysis

2. Course Contents:

This laboratory course will consist of experiments outlined below

1. Surface area determination of catalysts
2. determination of pore size distribution of catalysts
3. X ray diffraction and particle size determination
4. TPD measurements
5. Spectroscopic measurements (UV-Vis and FT-IR)
6. Chromatographic analysis
7. Preparation of zeolites
8. Studies of catalytic reactions using flow reactors
9. Optical resolution in analysis
10. Electrochemical measurements on catalysts
11. Chemical Analysis of supported and multi-component Catalysts – ICP, quantitative methods
12. Experiments in the use of high pressure reactors
13. Mechanical properties of catalysts

3. Text Books and 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.

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Preparation and properties of industrial catalysts</td><td>Course No.</td><td colspan="4">CA 531</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M. Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof S Sivasanker
Prof A V Ramaswamy
Prof. B Viswanathan</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">July 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

Catalyst preparation is a technology and fundamentals of this will be covered

2. Course Contents:

Classification of catalysts; requirements of industrial catalysts; general methods for preparation of catalysts: decomposition, precipitation, sol-gel, hydrothermal methods, leaching, impregnation, ion-exchange, hydrolysis, vapour deposition; unit operations: filtration, crystallization; activation of catalysts: calcinations, reduction, sulfidation; effect of preparation methods on catalyst activity; shaping of catalysts: importance of catalyst shapes, importance of heat and mass transport in industrial catalysis; reactor types; preparation of porous catalysts: oxides, mixed oxides; structure and preparation of zeolites, metallosilicates, aluminophosphates, ordered mesoporous materials; catalysis by zeolites; effect of Si/Al ratio, dealumination methods, crystallite size, Al-speciation; clay based catalysts, layered double hydroxides; structured catalysts: metal / ceramic monolith catalysts; composition analysis and simple characterization techniques for industrial catalysts; screening of industrial catalysts for activity and selectivity; reactor types and methods.

3. Text Books and References:

1. B.Delmon, P.Grange, P.A.Jacobs and G.Poncelet, Preparation of catalysts, Sceintific bases for the preparation of heterogeneous catalysts, Elasevier, Amsterdam, 1976,1979,1983,1987,1991,1995.
2. Preparation of solid catalysts, Eds. G. Ertl, H. Knozinger, J. Weitkamp. John Wiley and Sons Inc. (1999).
3. B.C. Gates, Catalytic Chemistry, John Wiley and Sons Inc. (1992).
4. C.N. Satterfield, Heterogeneous catalysis in industrial practice, McGraw-Hill, New York (1991)
5. R.L. Augustine, Heterogeneous catalysis for the synthetic chemist, Marcel Dekker Inc., New York, 1996.
6. B.C. Gates, J.R.Katzer and G.C.A.Schuit, Chemistry of catalytic processes, McGraw-Hill, 1979.
7. H.F. Rase, Handbook of commercial catalysts, CRC press, 2000.

DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Homogeneous Catalysis</td><td>Course No.</td><td colspan="4">CA 532</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td></td><td></td><td></td><td></td></tr>
<tr><td>Offered for</td><td>M. Tech (Catalysis Technology)</td><td>Status</td><td colspan="2">Core</td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof. A V Ramaswamy
Prof. P Selvam
Dr. D Chakraborty (to be invited)</td><td>Type</td><td colspan="2">New</td><td colspan="2">Modification</td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">July 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
<tr><td colspan="7">1. Objectives: Homogeneous catalysis and its role in industrial catalysis will be examined</td></tr>
<tr><td colspan="7">2. Course Contents:
Importance of homogeneous catalysis in the synthesis of high-value chemicals; Organo-metallics and importance of ligands; catalytic cycle and catalytic intermediates and their identification through spectral techniques.
Reactions that olefins undergo: hydrogenation and asymmetric synthesis; isomerization, oligomerization, hydrocynation and metathesis reactions; Examples of Shell and DuPont processes.
Carbonylation and hydroformylation reactions: methanol to acetic acid; carbonylation of alkynes and other substrates for making industrially important chemicals; regio-selective reactions; bi-phasic catalysis.
Polymerization: catalytic cycle for alkene polymerization; metallocene catalysts; structure, special features and stereocontrol by metallocene catalysts.
Oxidation reactions: Wacker oxidation; metal-catalyzed liquid phase oxidation of cyclohexane, p-xylene, epoxidation of propene; oxo complexes and mechanism of oxidation reactions</td></tr>
<tr><td colspan="7">3. Text Books and References:
1. G.W.Parshall and S.D.Ittel, Homogensous Catalysis, The applications and chemistry of catalysis by soluble Transition Metal Complexes, Wiley, New Yor, 1992.
2. B.Cornils and W.A.Herrmann, Applied Homogeneous catalysis with Organometallic Compounds, Vol 1 and 2, Weinheim, New York, 1996.
3. S.Bhaduri and D.Mukesh, Homogeneous Catalysis, Mechanism and Industrial Applications, Wiley, New York, 2000.
4. P.W.N.M.Van Leeuwen, Homogeneous Catalysis: Understanding the art, Kluwer, Academic Publishers, 2003.</td></tr>
</table>

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Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Bio Catalysis</td><td>Course No.</td><td colspan="4">CA 533</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof. B Viswanathan
Prof. Anju Chadha and Biotechnology faculty will be invited</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">July 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

Fundamentals of bio catalysis will be dealt with

2. Course contents:

Fundamentals: why these reactions exhibit special kinetics and examples; bio catalytic reactors; principles of catalysis in chemistry and biology; catalytic strategies, protein folding, structure and dynamics, from amino acids to three dimensional structure of proteins; methods for determination; concise review of protein folding; protein dynamics-activity relationship; Enzyme kinetics: Introduction to kinetics (steady state kinetics and pre-steady state kinetics); inhibition patterns as a mechanistic tool; isotope effects; enzyme-ligand interactions; thermodynamics and kinetics; cofactors, chemical function of various coenzymes; post-translational and chemical modifications; biogenesis and function of post-translational as derivatizations; chemical modifications; metals and electron transfer. Introduction to bioinorganic chemistry of enzymes; RNA catalysis; structure, function and applications; implication to evolution (RNA world), Catalytic antibodies; recent findings and their applications to bio-catalysis in general. Extremophiles: stability and function of enzymes evolved under extreme conditions; comparison to their mesophilic ("normal") analogues; implication to evolution (primitive enzymes?). Mechanistic examples, recent examples: the evolution of understanding mechanisms; Low - barrier hydrogen bond; concepts outside the main stream of enzymology. Synthetic and industrial uses. Enzymes in organic solvents; immobilized enzymes. Approaches in drug development, Enzyme engineering and biomimetic catalysts.

3. Text Books and References:

1. Laszlo Poppe and Lajos Novak, Selective Biocatalysis: A Synthetic Approach (1992)
2. Illanes Andrés (Ed.), Enzyme Biocatalysis, Principles and Applications , 2008,
3. Bommarius, Andreas S. / Riebel-Bommarius, Bettina R, Biocatalysis: Fundamentals and Applications, Wiley 2004.
4. W.D.Fessner (Editor) Biocatalysis: From Discovery to Application, Springer
5. T.Matsuda, Future directions in Biocatalysis,Elsevier
6. C.T.Hou, Biocatalysis and Bioenergy, Wiley interscience, 2008.

DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS
(NCCR)
Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Computational study of surfaces and catalysis</td><td>Course No.</td><td colspan="4">CA 534</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M. Tech Catalysis Technology</td><td>Status</td><td colspan="2">Core</td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Dr R Ramnarayanan
Prof P Selvam
Prof. B. Viswanathan</td><td>Type</td><td colspan="2">New</td><td colspan="2">Modification</td></tr>
<tr><td>Pre-requisite</td><td></td><td>To take effect from</td><td colspan="4"></td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

This course gives some computations methods for treating catalytic problems

2. Course Contents:

Schrodinger Equation and particle in a box, Operators, Harmonic Oscillator, Theorems of Quantum Mechanics, Variation Method, Perturbation Theory, Virial and Hellmann-Feynman Theorem, Molecular Symmetry and many electron atoms.

1. Electronic structure of atoms and Pseudopotentials, Plane waves and grids, localized orbitals and calculations, augmented functions
2. Periodic solids and electron bands, Bloch Theorem, Brillouin Zone, Uniform electron gas and simple metals, Hartree-Fock, Density Functional Theory: foundation, Functionals for electron and exchange correlation, Kohn-Sham ansatz and solution
3. Quantum Monte Carlo, Molecular Dynamics, Response and Wannier functions.
4. Surface structure, Adsorbate electronic structure and bonding on metal surfaces, The dynamic of making and breaking bonds at surfaces, Heterogeneous catalysis, Geochemistry, semiconductor surface chemistry

3. Text Books and References:

1. Computational Quantum Chemistry, Charles M Quinn, Academic Press, London, UK, 2002 with a CD. Available in the IITM library under Call No 541.27:519.6 QUI.
2. Electronic Structure: Basic Theory and Practical Methods, Richard M. Martin, Cambridge University Press, Cambridge, UK, 2004 and www.electronicstructure.org complementing the book.
3. Chemical bonding at surfaces and interfaces, Editor Editors: Anders Nilsson, Lars Pettersson, Jens Norskov, Elsevier, NewYork, NY 2008. Available in the IITM library under Call No 541.57 NIL.
4. Quantum Chemistry, 5th Edition, Ira N. Levine, Prentice Hall, 1999, NJ, USA.

5. Solid State Physics, Neil W. Ashcroft and N. David Mermin, Brooks/Cole, a Divison of Thomson Learning, India Edition, 2007.
6. Molecular Quantum Mechanics, 3rd Edition, P. W. Atkins and R. S. Friedman, Oxford University Press, Oxford, UK, 2004.
7. Course handouts and website links as and when appropriate. Some important websites and papers include:
    a) Basic Density Functional Theory at http://prola.aps.org/toc/RMP/v71/i5
    b) Time Dependent Density Functional Theory at http://dft.uci.edu/APSTutorial/literature.pdf
    c) Electronic structure - Activity correlations
    1. Electronic Structure and Catalysis on Metal Surfaces, Jeff Greeley, Jens K. Nørskov, Manos Mavrikakis, Annual Review of Physical Chemistry, 2002, 53, 319-348.
    2. Theoretical surface science and catalysis - calculations and concepts, B.Hammer and J.K.Norskov, Advances in Catalysis, 2000, 45, 71-129.
    d) Surface diffusion
    1. Recent Developments in the theory of Surface Diffusion, D Doll and A. F. Voter, Annual Review of Physical Chemistry, Oct 1987, 38, 413-431.
    2. Diffusion of adsorbates on metal surfaces, R. Gomer, Reports on Progress in Physics, 1990, 53(7), 917-1002.
    e) Monte Carlo methods
    1. Theoretical foundations of dynamical Monte Carlo simulation, K. A. Fichthorn and W. H. Weinberg, Journal of Chemical Physics, 1991, 95(2), 1090-1096.
    2. A general method for numerically simulating the stochastic time evolution of coupled chemical reactions, D. T. Gillespie, Journal of Computational Physics, 1976, 22(4), 403-434.
    3. A random-walk simulation of the Schrodinger equation: H3+, James B Anderson, Journal of Chemical Physics, 1975, 63(4), 1499-1503.

DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS

(NCCR)

Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Catalysis in Petroleum Technology</td><td>Course No.</td><td colspan="4">CA 535</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof. S Sivasanker
Prof. B Viswanathan</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4">July 2009</td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

Catalysis in Petroleum technology is an important area and this course examines the possibilities.

2. Course Contents:

Origin, composition of petroleum; production of different fuel fractions: refinery operations;primary processing, secondary processing, thermal and catalytic methods; analysis, tests and specifications for petroleum fuels; catalytic cracking: catalysts, processes; catalytic reforming: reactions, catalysts, processes; hydrodesulfurization (HDS) of fuel fractions, catalysts, active centres and mechanisms; deep desulfurization of diesel fuels; sweetening of kerosene, alternate desulfurization methods; desulfurization of FCC naphtha; hydrocracking: catalysts and processes; processing of heavy oils - hydrodemetallization, residue HDS; lube oil production – dewaxing, wax isomerization: catalysts and processes. alkylates for petrol – current processes, use of solid acids; light naphtha isomerization, catalysts and current processes; oxygenate additives; sulfur recovery from fuel processing operations; H_2-production; deactivation of catalysts; regeneration of catalysts; recovery of materials; types of reactors used in fuels processing.

3. Text Books and References:

1. J.G.Speight, The Chemistry and Technology of Petroleum, Marcel Dekker Inc., 1980
2. Meyers, R.A. (ed.), Handbook of Petroleum Refining Processes, Part 5, McGraw-Hill, New York (1986).
3. “The Chemistry and Technology of Petroleum”, J.G. Speight, (Marcel Dekker,1991).
J.F. Le Page et al., Applied Hetrogeneous Catalysis, (Editions Technip, Paris).
4. J. Scherzer and A.J. Gruia, “Hydrocracking Science and Technology”, Marcel Dekker, N.Y., 1996.
5. J.G. Speight, “The Desulfurization of Heavy Oils and Residua”, Marcel Dekker, N.Y., 1981.
6. A. Sequiera, Jr., “Lubricant Base Oil and Wax Processing”, Marcel Dekker, N.Y., 1994.
7. H. Topsoe, B.S. Clausen and F,E. Massoth, “Hydrotreating Catalysis: Science and Technology”, in Catalysis Science and Technology (eds. J.R. Anderson and M. Boudart) Springer Verlag, vol. 11, 1996.
8. “Catalytic Naphtha Reforming” (eds. G.J. Antos, A.M. Aitani and J.M. Parera) Marcel Dekker, 1995.
9. R.J. Farrauto and C. H. Bartholomew, Fundamentals of Industrial Catalytic Processes, Chapman and Hall, 1997.

DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS

(NCCR)

Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Catalysis in Production of Chemicals</td><td>Course No.</td><td colspan="4">CA536</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof S Sivasanker
Prof. P Selvam
Prof. A V Ramaswamy</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4"></td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

Chemical production is mostly catalysis based technology and hence the course examines the possibilities.

2. Course Contents:

Syngas production; preparation of pure hydrogen; ammonia synthesis, methanol and acetic acid; production of aromatics: p-xylene, ethylbenzene, cumene, styrene, alkyl benzenes; alkylation, dealkylation, trans alkylation and disproportionation; zeolite catalysis: structure of zeolites and principles of zeolite catalysts, shape selectivity; molecular sieve separation processes; production of monomers: olefins, caprolactam, vinyl chloride; selective oxidation reactions, ammoxidation, ammoximation; production of adipic acid, terephthalic acid, acrolein, acrylic and methacrylic acids, ethylene oxide and ethylene glycol, epichlorohydrin, phenol, formaldehyde, formic acid, propylene oxide, propylene glycols, acrylonitrile, vinyl acetate; ethanol, sulfuric acid, nitric acid, hydrogen peroxide; alpha-olefins and alcohols; olefin metathesis; green chemistry: green catalysts and processes, solid catalysts in organic synthesis, fine chemicals manufacture, metallosilicate catalysts for selective oxidations; solid catalysts for pharmaceuticals, enantioselective catalysis.

3. Text Books and References:

1. C.H. Bartholomew, Fundamentals of industrial catalytic processes, Chapman & Hall, 1997.
2. N.Y. Chen, W.E. Garwood and F.G. Dwyer, “Shape Selective Catalysis in Industrial Applications”, Marcel Dekker Inc., New York, 1989.
3. P.H. Spitz, Petrochemicals, the rise of an industry, John Wiley & Sons, 1988.
4. R.A. Meyers, Handbook of petrochemical production processes, McGraw-Hill, 2005.
5. Meyers, R.A. (ed.), Handbook of Petroleum Refining Processes, Part 5, McGraw-Hill, New York (1986).
6. S. Matar and L.F. Hatch, Chemistry of petrochemical processes, Butterworth-Heinemann, 2001.
7. R.L.Augustine, Heterogeneous Catalysis for the synthetic chemist, (1995)
8. C.H.Bartholomew and R J Ferrauto, Fundamentals of Industrial Catalytic Processes, 2005.
9. Ruud I. Wijngaarden, K. Roel Westerterp, and A. Kronberg, Industiral Catalysis: Optimizing Catalysts and Processes, 1998.
10. Howard F. Rase, Hand book of commercial Catalysts: Heterogeneous Catalysts, 2000.
11. Dennis Morrell, Catalysis of Organic Reactions (Chemical Industries), 2002.

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(NCCR)
Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Nano-materials and Catalysis</td><td>Course No.</td><td colspan="4">CA 537</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof. P Selvam
Prof. B.Viswanathan
Dr. R Ramnarayanan</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4"></td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

This is an emerging area and hence provides modern approach to the course.

2. Course Contents:

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 two-dimensional 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.

3. Text Books and References:

1. P. Yang (ed), The Chemistry of Nanostructured Materials, World-Scientific, 2003.
2. G. Cao, Nanostructures and Nanomaterials - Synthesis, Properties and Applications, World-Scientific, 2004.
3. G.A. Ozin and A.C. Arsenault, Nanochemistry: A Chemical Approach to Nanomaterials, RSC Publishing, 2005.
4. E. Roduner, Nanoscopic Materials: Size Dependent Phenomena, RSC Publishing, 2006.

DEPARTMENT OF CHEMICAL ENGINEERING, IIT MADRAS

(NCCR)

Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Catalysis in green chemistry and environmental applications</td><td>Course No.</td><td colspan="4">CA 538</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Prof. S.Sivasanker
Prof. A V Ramaswamy
Prof P Selvam</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4"></td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

Catalysis is necessary for cleaner environment. Green chemistry and environmental quality improvement are very important applications of catalysis

2. Course Contents:

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; 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.

3. Text Books and References:

1. P.T. Anastas and J.C.Warner, Green Chemistry, theory and practice,
2. M. Lancaster, Green chemistry, an introductory text, RSC, 2002.
3. G. Rothernberg, Catalysis: concepts and green applications.
4. R.J. Farrauto, Catalytic air pollution control, Van Nostrand Reinhold, New York, 1995.
5. R.J. Farrauto and C. H. Bartholomew, Fundamentals of Industrial Catalytic Processes, Chapman and Hall, 1997.
6. A. Matalack, Introduction to green chemistry, Marcel Dekker, 2001.
7. R.A. Sheldon, I.Arends, U. Hanefeld, Green Chemistry and catalysis, Wiley

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(NCCR)
Introduction of a New Course

<table>
<tr><td>Course Title</td><td>Photo-catalysis</td><td>Course No.</td><td colspan="4">CA 539</td></tr>
<tr><td rowspan="2">Department</td><td rowspan="2">Chemical Engineering (NCCR)</td><td rowspan="2">Structure</td><td>L</td><td>T</td><td>P</td><td>C</td></tr>
<tr><td>3</td><td>0</td><td>0</td><td>3</td></tr>
<tr><td>Offered for</td><td>M.Tech Catalysis Technology</td><td>Status</td><td colspan="2"></td><td colspan="2">Elective</td></tr>
<tr><td>Faculty</td><td>Dr. R. Ramnarayanan
Prof. P Selvam
Prof. B Viswanathan</td><td>Type</td><td colspan="2">New</td><td colspan="2"></td></tr>
<tr><td>Pre-requisite</td><td>Nil</td><td>To take effect from</td><td colspan="4"></td></tr>
<tr><td>Submission Date:</td><td>Date of approval by DCC:</td><td>Date of approval by BAC</td><td colspan="4">Date of approval by Senate</td></tr>
</table>

1. Objectives:

Catalysis is useful in harvesting the abundant solar energy. This is a potential application of catalysis.

2. Course Contents:

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.

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

Photoelectrochemistry : concepts, discoveries and applications, storage and synthetic cells, energy generation, cell design, diagnosis and characterization of photoprocesses at electrodes.

3. Text Books and References:

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
7. Course handouts and website links as and when appropriate.