

# CHEMICAL SCIENCES

*Programme Code:* CHEM04

*Programme Outcome:*

- Foundation in the fundamentals of core chemical sciences fields including those in Analytical, Inorganic, Nuclear and Physical Chemistry.
- Understand fundamental concepts across chemistry, materials science, nuclear science, and engineering disciplines relevant to research scholars
- Grasp synthesis, structure, and property relationships in inorganic, organic, and nuclear materials
- Apply theoretical and experimental chemistry, including spectroscopy, computational methods, and material characterization techniques
- Comprehend nuclear chemistry, radioactivity, nuclear reactions, nuclear models, and actinide chemistry fundamentals
- Understand the chemistry and technologies involved in the entire nuclear fuel cycle from mining to waste management
- Gain knowledge of production, applications, and safety aspects of radioisotopes
- Analyze interactions of radiation with matter and their implications
- Master principles, processes, and materials critical for nuclear reactors and fuel cycle processing systems
- Understand corrosion science and engineering with special emphasis on nuclear environments
- Develop skills in analytical chemistry, instrumentation, and laboratory techniques tailored to nuclear materials
- Acquire knowledge of health physics, radiation safety, and radiation monitoring principles
- Learn reactor physics, fuel design, and nuclear reactor system fundamentals
- Understand molecular spectroscopy and laser applications relevant to chemical and nuclear research
- Explore advanced topics in nanomaterials and chemical sensors for nuclear and energy applications
- Develop research aptitude, problem-solving, data analysis, and scientific communication skills for nuclear science and engineering

## DETAILED COURSE COURSES

CORE COURSE				
Sr. No	Course Code	Course Title	Hour(L)	Credits
1	CH1	Mathematics and computational methods	45	3
2	CH2	Chemical Thermodynamics	45	3
3	CH3	Electrochemistry	30	2
4	CH4	Introduction to Materials Science and Engineering	45	3
5	CH5	Analytical Chemistry for Nuclear Fuel Cycle	45	3
6	CH6	Chemical Instrumentation Laboratory Techniques	45	3
7	CH7	Health Physics and Radiation Sciences	45	3
8	CH8/MS4	Introductory Reactor Physics and Fuel Design	30	2
9	CH9	Chemistry of Fuel Cycle - I	45	3
10	CH10	Chemistry of Fuel Cycle - II	45	3
11	CH11	Materials for Nuclear Reactors and Fuel Cycle Processing systems	30	2
12	CH12	Nuclear & Radiochemistry	45	3
13	CH13/MS13	Corrosion science and Engineering	45	3
14	CH14	Quantum Chemistry and Group Theory	45	3
15	CH15	Molecular Spectroscopy	45	3
16	CH16	Lasers and Application	45	3
17	CH17	Nanomaterials and Advanced Chemical Sensors	45	3
		*Research Methodology & Research Publication Ethics	45	3
<b>Total</b>			<b>600</b>	<b>48</b>

*\*Research Methodology & Research publication Ethics (03 credits) course will be conducted by HBNI*

*\*\* 1 Credit is equivalent to 15 contact hours of classroom teaching as per the new UGC guideline.*

*\*\*\* 1 Credit is equivalent to 30 contact hours of Lab work/project as per the new UGC guideline.*

## CORE COURSES COORDINATOR

CORE COURSES			
Code	Course	Course Coordinator	
CH1	Mathematics and computational methods	Dr .Sundararajan	sundar@igcar.gov.in, Ext: 24152
		Dr .S S Ghosh	ssghosh@igcar.gov.in, Ext:24194
CH2	Chemical Thermodynamics	Dr .Rajesh Ganesan	rajesh@igcar.gov.in, Ext:24129
		Dr .Sham Kumar	shyam@igcar.gov.in, Ext: 24009
CH3	Electrochemistry	Dr .Sajal Ghosh	sajal@igcar.gov.in, Ext:24139
		Dr .A Sree Rama Murthy	asrm07@igcar.gov.in, Ext:24172
CH4	Introduction to Materials Science and Engineering	Dr .H N Jena	hnje@igcar.gov.in, Ext:24033
		Dr .K I Gnanasekaran	igsk@igcar.gov.in, Ext:24073
CH5	Analytical Chemistry for Nuclear Fuel Cycle	Dr .N Ramanathan	nram@igcar.gov.in, Ext:24096
		Dr .K C Pitichaiah	nani@igcar.gov.in , Ext:24340
CH6	Chemical Instrumentation and Laboratory Techniques	Dr.. Sundararajan	sundar@igcar.gov.in, Ext:24152
		Dr .Pavan Kumar Narayanam	pavankumarn@igcar.gov.in, Ext:24270
CH7	Health Physics and Radiation Sciences	Dr. S. Chandrasekar	schand@igcar.gov.in, Ext:23556
		Dr .O Annalakshmi	anna@igcar.gov.in , Ext: 23421
CH8/MS4	Introductory Reactor Physics and Fuel Design	Shri. D Naga Sivayya	dnsiva@igcar.gov.in , Ext:21232
CH9	Chemistry of Fuel Cycle – I	Dr. C V S Brahmananda Rao	brahma@igcar.gov.in , Ext:24160
		Dr. S Balakrishnan	balakrish@igcar.gov.in, 24024
CH10	Chemistry of Fuel Cycle - II	Dr.C V S Brahmananda Rao	brahma@igcar.gov.in , Ext:24160
		Dr. B Sreenivasulu	bsrinu@igcar.gov.in , Ext:24320

CH11	Materials for Nuclear Reactors and Fuel Cycle Processing systems	Dr. Rajesh Ganesan	rajesh@igcar.gov.in, Ext:24129
		Dr.. Pushpalatha	pushpa@igcar.gov.in, Ext: 23345
CH12	Nuclear and Radiochemistry	Dr.. Sundararajan	sundar@igcar.gov.in, Ext:24152
		Dr. G V S Ashok Kumar	gvs@igcar.gov.in , Ext:24030
CH13/MS13	Corrosion science and Engineering	Dr. S Ningshen	ning@igcar.gov.in , Ext: 22094
		Dr .C Jagadeeswara Rao	cjr@igcar.gov.in, Ext: 22046
CH14	Quantum Chemistry and Group Theory	Dr. N Ramanathan	nram@igcar.gov.in , Ext: 24096
		Dr .G Gopakumar	gopakumar@igcar.gov.in, Ext:24345
CH15	Molecular Spectroscopy	Dr. N Ramanathan	nram@igcar.gov.in, Ext:24096
		Dr .Satendra Kumar	sat@igcar.gov.in, Ext:24323
CH16	Lasers and Application	Dr .Satendra Kumar	sat@igcar.gov.in, Ext:24323
		Dr .Sajal Ghosh	sajal@igcar.gov.in, Ext:24139
CH17	Nanomaterials and Advanced Chemical Sensors	Dr .Pavan Kumar Narayanam	pavankumarn@igcar.gov.in, Ext:24270
		Dr .A Sree Rama Murthy	asrm07@igcar.gov.in, Ext:24172

## CORE COURSES

### CH1: Mathematical and Computational Methods (45L Hours) (02-CHEM04-601-C)

Coordinators: Dr. Sundararajan (sundar@igcar.gov.in),  
Dr. S S Ghosh (ssghosh@igcar.gov.in)

#### Course Details:

- **Differential Equations & Integral Transforms**

Linear differential equations: Series method of solution; Legendre, Lagurre and Hermite differential equations. Use of ladder operators for solutions to differential equations; applications to quantum chemistry. Orthogonal Polynomials and Special functions – Dirac Delta function, gamma function, error function. Introduction to Fourier series, Fourier transform and Laplace transform applications in quantum chemistry and spectroscopic techniques – FT-NMR, FT-IR. Convolutions of functions, use of Fourier transforms in convolution, Applications in chemistry.

- **Vectors**

Vector differentiation and integration: Concepts of gradient, divergence and curl and their physical significance. Orthogonal vectors, Gram-Schmidt process – applications in quantum chemistry. Vector fields in space – Gauss and Stokes theorem with applications.

- **Matrix Algebra**

Elementary operations and elementary matrices. Rotation matrices, Similarity transformations; Applications of numerical techniques in matrix algebra to evaluate eigenvalues and eigenvectors; Diagonalization and inversion of matrices. Applications in chemistry.

- **Numerical Methods**

Newton-Raphson method for finding roots, differentiation, integrations by quadrature techniques, solutions of differential equations

#### Course Outcomes:

- Develop a deep understanding of fundamental mathematical concepts and their application in solving complex problems.
- Acquire proficiency in computational techniques, including numerical methods, algorithmic problem-solving, and programming for mathematical analysis.
- Apply mathematical reasoning and computational tools to model, analyze, and interpret scientific and engineering phenomena.
- Gain hands-on experience in using software and computational approaches to investigate data, generate solutions, and communicate mathematical results effectively.

#### References:

1. Advanced Inorganic Chemistry by F. A. Cotton and G. Wilkinson
2. Introduction to Ligand Field by B. N. Figgis
3. Inorganic chemistry by Shriver & Atkins, 5th edition
4. Solid State Chemistry and its Applications by A.R. West, Wiley, 1989, 2nd edition, Singapore.
5. Principles of Bioinorganic Chemistry, Stephen J. Lippard, Jeremy Mark Berg, Univ Science Books, CA.

## CH2: Chemical Thermodynamics (45L Hours) (02-CHEM04-602-C)

Coordinators: Dr. Rajesh Ganesan (rajesh@igcar.gov.in),  
Dr. Sham Kumar (shyam@igcar.gov.in)

### Course Details:

- **Laws of Chemical Thermodynamics**

Thermodynamic laws, thermodynamic properties of the system, criterion for equilibrium, Heat engines, Helmholtz energy, Gibbs energy, closed system, Maxwell's equations, Gibbs-Helmholtz equation.

- **Behaviour of Gases**

Gas laws, ideal gas and deviations from ideality, Vander Waal's equation, equation of state, critical phenomena, Thermodynamic treatment of non-ideal gases, gas mixtures. Raoult's and Henry's laws, activity of a component in solution, Gibbs-Duhem properties of Raoultian ideal solutions, Colligative properties, Non ideal and regular Partial and Integral thermodynamic property evaluation, alpha function, Gibbs free formation of regular solutions, Criteria for stability of regular solutions, Miedema's solution model, sub-regular solutions, Models for ternary systems.

- **Phase Equilibria**

Phase rule, Gibbs Free energy as a function of temperature and pressure, Equilibrium between a vapor and a condensed phase in a single component system, Graphical representation of phase equilibria in a single component system, Gibbs energy and thermodynamic activity, phase diagrams- single component, binary and ternary diagrams, simple calculation of thermodynamic properties from phase diagram, pressure-composition diagrams, CALPHAD and models for optimization of phase diagrams.

- **Reactions in Gases and Condensed Phases**

Reaction equilibria in homogeneous and heterogeneous media, effect of temperature and pressure on equilibrium constant, Le Chatelier's principle, Reaction equilibria in H<sub>2</sub>/H<sub>2</sub>O, CO/CO<sub>2</sub> systems, Ellingham diagrams, Effect of phase transformation, use of different standard states for representing reactions in condensed phases, phase stability diagrams, application of phase diagrams in material systems.

- **Statistical Thermodynamics**

Entropy and disorder in an atomic scale, concept of microstate, most probable microstate, influence of temperature, Boltzmann equation, partition functions, configurational entropy and thermal entropy.

- **Experimental Thermodynamics**

Calorimetry - classification of calorimeters, different types of calorimeters, heat capacity measurements, thermochemical calorimetry, estimation of thermodynamic quantities.

Vapor pressure measurements- static methods, transpiration, boiling point method, isopiestic method, Knudsen effusion method, Langmuir evaporation method, role of mass spectrometry for study of vaporization reactions, second and third law methods, Gibbs energy functions from spectroscopy data, measurements at very high temperatures.

Galvanic cell EMF methods for activity measurements, - solid electrolyte and molten salt EMF methods. Measurement of oxygen and carbon potentials – gas equilibration/ EMF methods. Determination of phase diagrams- spot technique, thermal analysis, enthalpies of transformations, transformation temperature, order of transformation, DTA, TGA, thermal expansion, resistivity- as a function of temperature, thermal diffusivity, measurement of thermal diffusivity and thermal conductivity.

**Course Outcomes:**

- Understand the fundamental laws and concepts of thermodynamics, including thermodynamic variables, functions, and their practical significance.
- Apply thermodynamic principles to analyze and solve problems related to energy changes, phase equilibria, and chemical equilibria in physical and chemical systems.
- Evaluate thermodynamic properties of pure substances and mixtures, and assess criteria for equilibrium and spontaneity of chemical processes.
- Develop quantitative and analytical skills to model thermodynamic behavior, interpret experimental results, and critically assess uncertainty in thermodynamic measurements.

**References:**

1. Physical Chemistry, G W Castellan, Addison Wesley, 1971
2. Introduction to Metallurgical Thermodynamics, David R Gaskell, McGraw Hill, 1973
3. Physical Chemistry, P W Atkins, 7th Ed, Cambridge University Press, 2004.
4. Principles of Chemical Equilibrium with Applications in Chemistry and Chemical Engineering, K Denbigh, Cambridge University Press, 1981.
5. Chemical and Process Thermodynamics, 2nd Ed, B G Kyle, Prentice Hall, 1992.
6. Thermodynamics, G N Lewis, M Randall, revised by K S Pitzer and L Brewer, McGraw Hill, 1961.
7. Differential Scanning Calorimetry: An Introduction for Practitioners, G W H Hohne, Springer Verlag, 1996.
8. Characterization of high temperature vapours, Ed by J L Margrave, John Wiley, New York, 1967.
9. Physicochemical Measurements in Metal Research, Ed by R F Bunshah, Wiley, Interscience , New York, 1970.

### CH3: Electrochemistry (30L Hours ) (02-CHEM04-603-C)

Coordinators: Dr. Sajal Ghosh (sajal@igcar.gov.in),  
Dr. A Sree Rama Murthy (asrm07@igcar.gov.in)

#### Course Details:

- **Electrolytes**  
Different electrolyte systems (aqueous, ionic melts and solid electrolytes) and their conductivities; Debye-Huckel theory, Techniques for measuring electrical conductivities - DC and AC techniques.
- **Electrochemical Cells**  
Electrochemical potentials, Nernst equation and electrochemical series, Molten salt and solid electrolyte based cells.
- **Electrode Processes and Kinetics**  
Diffusion layers & characteristics of the diffusion layers, over potentials, Butler-Volmer and Tafel equations, polarisable and non-polarisable electrodes, reference electrodes, voltammetric techniques, polarography, Cyclic Voltammetry, rotating electrodes and micro-electrodes, chronopotentiometric and chronoamperometric techniques, elucidation of mechanisms of electrochemical reactions.
- **Applications of Electrochemical Principles**  
Electro-analytical techniques and electrochemical sensors; energy conversion and storage systems (fuel cells and batteries including metal hydrides); thermochemical data measurements.

#### Course Outcomes:

- Understand core electrochemical concepts such as electrode potentials, redox reactions, and the operation of various electrochemical and galvanic cells.
- Apply theoretical principles to analyze cell parameters, Nernst equation, over potentials, and kinetics of electrode reactions.
- Develop skills in experimental methods, including potentiometric and conductometric techniques, and use these to investigate electrochemical systems.
- Evaluate applications of electrochemistry in energy storage, corrosion, industrial processes, and environmental and biological systems.

#### Reference:

1. Electrochemical Methods: Fundamentals and Applications, AJ Bard & LR Faulkner, Wiley, New York, 1987.
2. Electrode Dynamics, AC Fisher, Oxford University Press, Oxford, 1996.
3. Electrochemistry, P.H. Reiger, Prentice-Hall International, Englewood Cliffs, 1995.
4. Solid electrolytes and their Applications, (Ed) E.C.Subba Rao, Plenum, New York, 1980.
5. Electrochemistry, C. M. A. Brett and A. M. O. Brett, Oxford University Press, 1993.
6. Laboratory Techniques in Electroanalytical Chemistry, 2nd Ed., by P. T. Kissinger and W. R.Heineman, Marcel Dekker, 1996.
7. Chemical Sensor Technology, Vol.2, (Ed) T. Seiyama, Kodansha Ltd., Tokyo, 1989
8. Chemical Sensor Technology, Vol.3, (Ed) N.Yamazoe, Elsevier, Amsterdam, 1991.
9. Solid State Gas Sensors, P.T.Mosley and B.C.Toefield, Adam Hilger, Bristol, 1987.
10. Advances in Electroanalytical Chemistry, Vol.2, A.J.Bard, Macel Dekker, New York, 1967.

## CH4: Introduction to Materials Science and Engineering (45L Hours) (02-CHEM04-604-C)

Coordinators: Dr. H N Jena ([hnje@igcar.gov.in](mailto:hnje@igcar.gov.in)),  
Dr. K I Gnanasekaran ([igsk@igcar.gov.in](mailto:igsk@igcar.gov.in))

### Course Details:

- **Structure, Bonding & Defects in Solids**

Single crystal & polycrystalline materials, Unit cell, Crystal symmetry, Bravais lattices, point groups & space groups, Miller indices, Cohesive forces in crystals, Madelung energy and its calculation for NaCl and CsCl, Crystal structures, Close packing, Ionic Radii and Radius ratios, Common crystal structures of elements & compounds, Factors influencing crystal structures, Structure-property relations, Defects in solids, Thermodynamics of defect formation, Non-stoichiometry, Ionic conduction, Solid electrolytes.

- **Diffraction Techniques**

Diffraction phenomenon, X-ray, neutron and electron diffraction, Bragg's Law, Size and shape of unit cell, Basics of crystal structure determination, Powder diffraction and single crystal methods, Phase identification by XRD, Powder diffraction data base, Indexing of diffraction patterns and lattice parameter calculation, Rietveld refinement, Particle size & residual stress determination by XRD.

- **Microstructure & Microscopy**

Microstructure - origin and significance, Optical and electron microscopy

- **Physical Properties**

Mechanical properties, Fracture, Strengthening mechanisms, Thermal expansion, Thermal conduction, Thermoelectric effects, Electrical and magnetic properties - metals, semiconductors and insulators, Band picture of solids, Ferroelectric materials, Superconductors, Magnetic properties, Magnetic domains, Optical properties, Non-linear optical properties, Lasers, Fibre optics & applications.

- **Chemical Reactivity of Solids**

Factors affecting chemical reactivity, Diffusion, Surfaces of solids, Surface analysis techniques –ESCA, Materials at very low and high temperatures, Materials under pressure, Radiation damage in solids, Corrosion.

- **Synthesis of Materials**

Solid state reactions, Wet chemical reactions and precursor techniques, Combustion synthesis, Sol-gel process, Soft chemical reactions, Crystal growth techniques with examples, Thin films, Nanocrystalline materials, Sintering.

- **Phase Diagrams & Phase Transformations**

Phase diagrams – significance, experimental & computational methods of phase diagram determination, Classification of phase transformations, Order-disorder transitions, Nucleation and growth theory, diffusion- controlled and diffusionless transformations, Thermal analysis techniques.

**Course Outcomes:**

- Understand the fundamental concepts of material structure, properties, and classification including metals, ceramics, polymers, and composites.
- Analyze the relationships between microstructure, processing, and properties of materials for engineering applications.
- Apply principles of crystallography, phase diagrams, and materials characterization techniques.
- Evaluate materials selection criteria for nuclear and other industrial applications with emphasis on performance and sustainability.

**Reference:**

1. Materials science and technology: a comprehensive treatment, (18 Vols.) Ed. R.W. Cahn, P. Haasen and E.J. Kramer, VCH, Weinheim, 1991.
2. Encyclopedia of materials: science and technology, (11 Vols.) K.H.J. Buschow et al., Elsevier, Amsterdam, 2001.
3. Introduction to solid state physics, C. Kittel, VII Ed, John Wiley & Sons, 1996.
4. Solid state chemistry and its applications, A.R. West, John Wiley & Sons, 1984.
5. The structure and properties of materials, (4 Vols.) Ed. J. Wulff, Wiley Eastern, 1974.
6. Materials science and engineering: an introduction, V Ed, W.D. Callister, John Wiley & Sons, N.Y., 2003.
7. Introduction to materials science and engineering, K.M. Ralls, T.H. Courtney and J. Wulff, Wiley Eastern, 1978.
8. Elements of x-ray diffraction, B.D. Cullity, Addison – Wesley, 1978.
9. Analytical chemistry by open learning: X-ray methods, C. Whiston, John Wiley & Sons, 1987.
10. X-ray diffraction: a practical approach, C. Suryanarayana and M. Grant Norton, Plenum, 1998.
11. The science and engineering of materials, IV Ed D.R. Askeland and P.P. Phule, Brooks/Cole, 2003.
12. The physics and chemistry of materials, J.I. Gersten and F.W. Smith, John Wiley & Sons, 2001.
13. Metallic materials: physical, mechanical and corrosion properties, P.A. Schweitzer, Marcel Dekker, 2003.
14. Introduction to Solids, L.V. Azaroff, Tata McGraw-Hill, Bombay, 1960.
15. Materials science and engineering: a first course, III Ed V. Raghavan, Prentice Hall of India, 1996.
16. Understanding materials science: history, properties, applications, R.E. Hummel, Springer Verlag, N.Y., 2004.
17. Crystal growth: processes and methods, P. Santhana Raghavan and P. Ramasamy, KRU Publications, Chennai.
18. Preparative methods in solid state chemistry, P. Hagenmuller, Academic, 1972.
19. Thin film deposition: principles and practice, D.L. Smith, McGraw-Hill, 1995.
20. Properties of materials, M.A. White, Oxford Univ. Press, 1999.

## CH5: Analytical Chemistry for Nuclear Fuel Cycle (45L Hours) (02-CHEM04-605-C)

Coordinators: Dr. N Ramanathan (nram@igcar.gov.in),  
Dr. K C Pitichaiah (nani@igcar.gov.in)

### Course Details:

#### ▪ Instrumental Methods – Principles and Applications

##### • Spectrochemical Methods

Radioactivity, Ionizing radiation, Radiation quantities and units, Basis and structure of the system for radiation protection, System of radiological protection for human, natural radiation.

##### • Mass Spectrometry

Interaction of radiation with matter, External and internal radiation hazards in nuclear and radiation facilities, Radiation dosimetry: basics, concepts and definitions, External radiation dosimetry and dosimetry of internally deposited radio nuclides, Radiation detection principles, Monitoring instruments and Personnel monitoring devices

##### • Thermal Methods

Exposure situations as per ICRP-103 recommendations, Control of external and internal radiation hazards, Radiation dose limits and its basis, General principles and techniques of radiation monitoring, air activity and area contamination, Assessment and control of radiation hazards in nuclear fuel cycle facilities with special reference to metallurgical, radiochemical and radioisotope facilities and fuel reprocessing plants, Criticality safety aspects, Environmental safety aspects during operation of nuclear and radiation facilities, Industrial hygiene and safety aspects during operation of nuclear and radiation facilities.

##### • Nuclear Methods

Safety aspects of design of radiochemical laboratory, its types and operational aspects, Partial containment/confinement systems and ventilation system in a laboratory.

##### • Separation Techniques – Principles and Applications

Safety aspects of design of radiochemical laboratory, its types and operational aspects, Partial containment/confinement systems and ventilation system in a laboratory.

##### • Ion Exchange: Conventional Membranes

Safety aspects of design of radiochemical laboratory, its types and operational aspects, Partial containment/confinement systems and ventilation system in a laboratory.

##### • Statistical Methods in Chemical Analysis

Safety aspects of design of radiochemical laboratory, its types and operational aspects, Partial containment/confinement systems and ventilation system in a laboratory.

▪ **Laboratory Experiments (any 5)**

- Determination of trace impurities in high purity materials by AAS
- Application of Electroanalytical Methods to trace analysis
- TGA and DTA study of inorganic compounds
- Neutron Activation Analysis of trace constituents in a complex matrix
- Analysis of an alloy sample by EDXRF
- Anion analysis by ion selective electrode.
- Chromatographic separation and measurement of the components in mixture Isotopic Analysis by Mass Spectrometry.

**Course Outcomes:**

- Understand analytical techniques and instrumentation applied in nuclear fuel cycle chemistry.
- Gain proficiency in sample preparation, qualitative and quantitative analysis of nuclear materials.
- Develop skills in radiochemical separation and isotopic analysis relevant to nuclear materials.
- Apply quality control and safety protocols specific to nuclear analytical chemistry.

**Reference:**

1. Fundamentals of Analytical Chemistry, D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, 8<sup>th</sup> Edition, Thomson (2004).
2. Principles of Instrumental Analysis, D.A. Skoog, F. J. Holler, T. A. Niemann, 5<sup>th</sup> Edition, Saunders College Publishing (1998).
3. A text book of Quantitative Analysis, A.I. Vogel, 5<sup>th</sup> Edition Revised by G. H. Jeffery, J Bassett, J. Mendham and R. C. Denney, ELBS (1989).
4. Statistics for Analytical Chemistry, J. C. Miller and J. N. Miller, 2<sup>nd</sup> Edition, Wiley (1998)

## CH6: Chemical Instrumentation and Laboratory Techniques (45L Hours) (02-CHEM04-606-C)

Coordinators: Dr. Sundararajan (sundar@igcar.gov.in),  
Dr. Pavan Kumar Narayanam (pavankumarn@igcar.gov.in)

### Course Details:

- **Passive Circuit Elements and Configurations**

Circuit behaviour of resistors, inductors and capacitors; the potential divider and the wheatstone Bridge (resistive and capacitive), R- L-C- circuits as filters and resonance circuits.

- **Electronic Devices and Their Role in Power Conversion and Amplification**

The junction diode, SCR, triacs and their role in rectification and AC power control; bipolar transistor and IGBT and their role in linear/switched mode power supplies and in amplification of signals; constant current power supplies Inverter circuits; issues in measurement of signals - Concept of input impedance and the role of J-FETs and MOSFETs

- **Operational Amplifiers and their Various Functionalities**

The basic OP-AMP and its desired characteristics; the inverting amplifier, the non-inverting amplifier, summing configuration; The differentiator and integrator circuits; comparator; precision rectifier; waveform generation.

- **Fundamental Issues Related to Chemical Instrumentation**

Role of chemical instrumentation in the nuclear fuel cycle, with relation to selectivity, sensitivity and automation amenability. The basic anatomy of excitation with energy source-interaction with analyte-detection of the effect produced; issues related to selectivity; sensitivity and detection limits; sources of noise and measures to minimize the effect; boxcar integrator, lock-in-amplifier

- **UV-VIS-IR Instruments**

Phenomenon of resonant absorption and Beer's law of photometry; implementation of Beer's law in a spectrophotometer; compensation for spectral response of the detector; slit servo mechanism for compensation of optical emission. Atomic absorption spectrophotometer-flame ionization, compensation for molecular absorption, hollow cathode lamp excitation for high specificity. Atomic emission spectrometry-principles, instrumentation and data interpretation. Laser fluorescence spectrometry-laser basics, three stage power supply for flash lamp excitation. Non dispersive spectrometer- FTIR - principle, data collection scheme.

- **X-Ray Spectrometry**

Generation of X-Rays, The X-Ray tube, setting the energy and intensity; Bragg's law; X-Ray fluorescence, X-Ray diffraction, ESCA for surface analysis. Mass Spectrometry: Ion sources-thermal ionization, Knudsen effusion and electron impact ionization, inductively coupled plasma source, Laser induced vapourisation, spark source. Magnetic analysers, quadrupole analyzers, time-of-flight analysers. Detectors faraday, SEM, Channeltron. Mass scanning, peak centering, signal handling and digitization and counting.

- **Thermal Analysis**

Thermal excitation - furnaces, temperature profiling and furnace power control. Thermal effects - TGA, DTA, DSC, dilatometry. Thermal measurements - thermocouples, RTDs, signal conditioning and handling. Additional Methods of Analysis: Gas chromatography - mobile and stationary phases; separation on the basis of retention time; TCD and FID detectors. Instrumentation for pH meters and conductivity meters; automated titro-processors and applications of coulometry. Radioactive assay based on multi-channel gamma-ray spectrometry.

- **Digital Electronics**

Logic gates; flipflops, counters, astable and monostable multivibrators; decoders; logic families; data conversion-various types of ADCs and DACs. Microprocessor systems-processor architecture, memory circuits, I/O subsystems; interfacing techniques; assembly language programming.

- **Laboratory Techniques**

Machine Drawings Projections: orthographic – 1st & 3rd Angles pictorial; Oblique: Perspective. Conventional representation of common features and sections; Dimensioning and tolerancing; Scales, lines and lettering; Threads; Fastenings.

Brief Introduction of AutoCAD and its use, common drawing and edit commands.

Vacuum systems - equipment for vacuum generation - rotary pumps, diffusion pumps, ion pumps, turbo molecular pumps; Generation of high temperatures, measurement of vacuum and temperatures, centrifuges, chemicals and laboratory safety.

Vacuum Generation and measurements: Kinetic theory of gases – Velocity distribution -Mean free path – Monolayer formation – vacuum units – Viscous and molecular Flow regimes – Reynold's and Knudsen Numbers viscosity and thermal conductivity of gases. Gas release from solids – vaporization – out gassing – diffusion – permeation – Vacuum pumps – Titanium Sublimation pumps – Ion pumps – Cryogenic pumps and matters for construction of Vacuum chamber. Gauges: Thermal conductivity, cold cathode, hot cathode ionization gauges and their principle of operation.

**Course Outcomes:**

- Master operating principles and applications of instrumental techniques such as spectroscopy, chromatography, and electrochemical analysis.
- Develop practical skills in experimental design, data collection, and interpretation of instrumental data.
- Gain hands-on experience with analytical instruments and laboratory safety procedures.
- Apply instrumental methods to real-world chemical and nuclear research problems.

**Reference:**

1. Principles of Instrumental Analysis, D. A. Skoog and J. Leary, McMillan Publishers,
2. Instrumental Methods of Analysis, H. H. Willard, L. L. Merritt, Jr., J. A. Dean, F. A. Settle, Jr. CBS Publishers and Distributors, New Delhi 1986.

## CH7: Health Physics and Radiation (45 Hours / 3 Credit) (02-CHEM04-607-C)

Coordinators: Dr. S. Chandrasekar (schand@igcar.gov.in),  
Dr. O Annalakshmi (anna@igcar.gov.in)

### Course Details:

#### ▪ **Interaction of Radiation With Matter**

Ionization in gaseous medium, Bragg's curve, stopping power, Bethe equation, range of particles and straggling, LET, attenuation and absorption of beta particles, backscattering, photoelectric, Compton and pair production processes for gamma radiation, variation with gamma energy and Z of medium, attenuation and absorption of gamma rays, elastic and inelastic scattering of neutrons.

#### ▪ **Radiation Detection and Measurement**

Principles of radiation detectors, counting characteristics, detection efficiency and energy resolution, dead time and counting statistics, Gas filled detectors, scintillation processes and detectors, organic and inorganic scintillators, NaI(Tl), LaBr<sub>3</sub>, semiconductor detectors, p-n junctions, germanium and silicon detectors, room temperature semiconductors, neutron detectors including bubble detectors, solid state nuclear track detectors, nuclear probes - positron annihilation, perturbed angular correlation, Mossbauer effect.

#### ▪ **Shielding and Dose Calculations**

Shielding (beta, gamma and neutron sources). Shielding from mixed sources; calculation of dose for point, line and volume sources. Dosimetry: Definition of various dosimetric terms (exposure, absorbed dose, equivalent dose, effective dose, concept of radiation and tissue weighting factors and their importance, Activity, Specific activity (SI units and Old units), radiological, biological and effective half- life and their relation and the concept of the same and their importance. Concept of ALI and DAC.

#### ▪ **Radiation Protection Principles**

Radiation protection philosophy, objectives and principles of radiation protection, Dose limits to occupational workers and members of public, Dose constraints, Investigation limits. Types of exposure (natural, occupational, medical and public). External and internal exposures; routes of intake of radioactive material. Use of personal dosimeters (Film badge, TLDs, pocket dosimeters). Calculation of internal dose, Exposure measurement: Free air and Air wall chambers (concept of wall thickness should be given), exposure-dose relationship, Bragg-Gray principle. Fundamentals of ICRP respiratory model, entry through ingestion, GI track model, whole body counting and bioassay techniques.

#### ▪ **Radiation Protection Procedures**

Procedures followed in radiation work places, supervised and controlled areas, work permits, contamination control methods (air-borne, surface and personnel), swipe samples, and rubber areas, spill pack (gloves + absorbing paper), decontamination and de-corporation techniques; bore wells and inspection chambers; precautions during radioactive source storage and handling. Types of radiation monitors / radioactivity measurement methods adopted for radiation protection. Personnel monitoring, area monitoring and stack monitoring.

#### ▪ **Waste Management**

Radioactive waste classification and management – An overview

- **Emergency Preparedness**  
Nuclear accidents, emergency preparedness and management: reasons for accidents, classification of accidents, International Nuclear Event Scale, types of emergency, emergency preparedness, counter measures.
- **Nuclear Fuel Cycle Applications**  
Radiological aspects and environmental impact of FBRs. Criticality safety and Radiological aspects in nuclear cycle facilities.
- **Regulatory Details**  
Atomic Energy Act, National and International regulatory bodies, their role and responsibilities, Radiation Protection Rules, Nature of duties and responsibilities of Radiation Safety Officer / Health Physicist, radio toxicity and classification of laboratories, design of lab for radioactive work, Safe handling of radioisotopes, Transport of radioactive materials.
- **Basic Radiobiology**  
Interaction of ionizing radiation with living cells, Ionizing radiations, excitation and ionization process, basic structure and components of cell, chemical and biological consequences of radiation action, radicals and reactions in cell killing, direct and indirect effect and relevant biological damage.
- **Molecular and Cellular Effects of Radiation**  
Radiation action and organizational level in cell, Damage to DNA, single and double structural breaks in units membrane dose and survival curve, cellular radioactivity, radiobiological effectiveness and linear energy transfer Dzz dose, rate effect, dose fractionation, Mitotic delay, chromosome aberration and mutations by radiation action on cells.
- **Modification of Biological Effects of Radiation**  
Oxygen effect, OER, Chemical radio sensitizers, Chemical radio protectors, Mechanisms of action and importance in nuclear research programme.
- **Radiobiology and Radiotherapy**  
Radiation and cancer, cell cycle and radiosensitivity, rationale of using radiation for tumor cell kill, problems.
- **Basics of Radiation Chemistry**  
Interaction of high energy radiation with matter, G-values, radiation induced reactions in solids, liquids and gases.
- **Laboratory Experiments (any 5)**
  - Plancheting, alpha counting and spectroscopy
  - Counting characteristics of gas detectors
  - Half life determination and attenuation coefficient determination
  - High resolution gamma spectrometry
  - Dose Measurements: Whole Body Counting laboratory, Bio-dosimetry laboratory, TLD personnel monitoring services laboratory.

▪ **Demonstrations**

- Use of Personnel Protective Equipment (PPE): Proper checking and wearing of gloves, and other plant dresses (shoe covers, boiler suits, overcoats etc.). Respirators (dust, gas mask, self-contained breathing apparatus, and fresh air- line) TLD, Film badge, neutron film, criticality badge and bubble detector.
- Use of Radiation Monitoring Equipment: Installed and Portable Radiation Monitors: AGM (audio and visual alarm, setting up of alarm limits); staplex air sampler (estimation of air-borne activity-both alpha and beta-gamma), different types of survey meters (low to high range), ALSCIN and GM based contamination monitors (side window and end window, hand and foot monitor, cloth monitor), continuous air monitor, criticality alarm system.

**Course Outcomes:**

- Understand principles of radiation interaction with matter and biological systems.
- Apply radiation protection standards, dosimetry, and safety measures in nuclear and medical environments.
- Evaluate health physics instrumentation and monitoring techniques for radiation detection.
- Develop skills in radiation risk assessment and management strategies.

**Reference:**

1. Introduction to Health Physics by Herman Camber
2. Biological Effects of Radiation by J. E. Coggle
3. Radiobiology for Radiologist by Eris J. Hall
4. Detection and Measurement of Radiation - Glenn T Knoll.

## CH8: Introductory Reactor Physics and Fuel Design (30L Hours)

Coordinators: Shri. D Naga Sivayya (dnsiva@igcar.gov.in),

### Course Details:

- **Basic Nuclear Physics Concepts**  
Properties of nuclei. Nuclear forces, Nuclear models. Nuclear decay, Liquid drop model and nuclear stability, Nuclear reactions including fission, Compound nucleus formation, Microscopic cross-section, Partial and total cross-sections.
- **Basics Neutron Physics Concepts**  
Introduction to physics of fission process. Definition of flux current and sources, Neutron-nuclear interaction cross sections, Reaction rate density, macroscopic cross section and mean free path. Cross-sections of elements, compounds and mixtures.
- **Chain Reaction: four factor formula**  
Definitions of k-infinity, k-effective w.r.t. neutron balance equation (with diffusion approximation); boundary conditions; definition of reactivity; criticality.
- **Homogeneous Reactor**  
Space dependence of neutron flux. Flux shape in different geometries, Slab/cylinder/spherical reactor, Geometric and material, buckling. Diffusion length, reflected slab, reflector saving. Heterogeneous reactors; typical examples.
- **Reactor Kinetics**  
Time dependent diffusion equation, Point kinetics, Prompt neutrons, Delayed neutron precursors, Reactor period, period versus reactivity, Inhour formula, one group delayed neutrons, one dollar of reactivity, Prompt and delayed criticality. Feed back coefficients.

### Course Outcomes:

- Comprehend basic reactor physics concepts including neutron behavior, criticality, and reactor kinetics.
- Understand fuel design principles, materials selection, and fabrication processes.
- Analyze reactor core components and their influence on neutronics and thermal performance.
- Utilize computational tools for reactor physics simulations and fuel cycle analysis.

### References:

1. The Elements of Nuclear Reactor Theory, Samuel Glasstone and M.C. Edlund. Van Nostrand, 1952.
2. Introduction to Nuclear Reactor Theory, Lamarsh J.R., ANS, 2002
3. Physics of Nuclear Reactors, Jakeman D., English Universities Press, 1966.
4. A.E. Walter and A.B. Reynolds, "Fast Breeder Reactors", Pergamon Press, 1981.

## CH9: Chemistry of Fuel Cycle –I (45L Hours) (02-CHEM04-609-C)

Coordinators: Dr. C V S Brahmananda Rao (brahma@igcar.gov.in),  
Dr. S Balakrishnan (balakrish@igcar.gov.in)

### Course Details:

- Recovery of the starting compounds bearing U, Pu or Th from their primary and secondary sources. Mining, beneficiation, pre-concentration, purification and recovery.
- **Oxide Fuels**  
Preparation of UO<sub>2</sub>, PuO<sub>2</sub>, MOX and ThO<sub>2</sub>. Physical and chemical properties, phase diagrams of relevance, control of phase composition and stoichiometry, fuel fabrication flow sheet and quality control
- **Advanced Ceramic Fuels**  
Carbides U-C, Pu-C, U-Pu-C, U-Pu-C-O and U-Pu-C-O-N, Nitrides U-N, Pu-N, U-Pu-N. Physical and chemical properties, phase diagrams of relevance, control of phase composition and stoichiometry, fuel fabrication flow sheet and quality control.
- **Advanced Fuel Fabrication Techniques**  
Oxides, Methods based on sol-gel and novel techniques. Carbides; sol-gel method, direct pressing and arc casting. Preparation of U, Pu and Th. Alloy Fuels: Historical over view of the alloy fuel development, alloys (U-Zr, U-Pu-Zr, U-RM, U-Pu- MA), dispersions and composites – Salient physical and chemical properties, relevant phase diagrams, fabrication and quality control.
- **Inert Matrix Fuels for Partitioning and Transmutation**  
A brief account on the current developments.
- **Fuel – Clad Interaction**  
Significance of FCCI and FCMI. Specifics pertaining to oxide, carbide and metallic fuels. Role of chemical thermodynamics in the prediction and understanding of Fuel clad chemical compatibility.
- **In Pile Behaviour of Fuels**  
Chemistry and redistribution of fission products, role of chemical potentials of the constituents in the breach of clad in oxide, carbide and alloy fuel pins and detection mechanisms.

### Course Outcomes:

- Understand chemical processes involved in nuclear fuel fabrication and reprocessing.
- Develop knowledge of thermodynamics and kinetics related to fuel cycle chemistry.
- Analyze chemical transformations in nuclear fuel during irradiation and handling.
- Apply radiochemical methods for fuel cycle process optimization and waste management.

### References:

1. Donald R. Olander, Fundamental aspects of nuclear reactor fuel elements fundamental aspects of nuclear reactor fuel elements, Springfield, BTIS, 1985.
2. H. J. Matzke, Science of Advanced LMFBR fuels, North Holland, Amsterdam, 1986.
3. M. Benedict and T.H. Pigford, Nuclear Chemical Engineering, Mc Graw Hill, New York, 1957.  
(Specific journal articles and other references will be cited during the lectures)

## CH10: Chemistry of Fuel Cycle –II: Actinide chemistry and separation science (45L Hours) (02-CHEM04-609-C)

Coordinators: Dr. C V S Brahmananda Rao (brahma@igcar.gov.in),  
Dr. B Sreenivasulu (bsrinu@igcar.gov.in)

### Course Details:

#### ▪ Actinide Chemistry

Discovery of actinide elements, electronic structure, oxidation states, inter-conversion of oxidation states, complexes of actinide ions, actinide contraction, comparison of actinides with lanthanides. Actinides in environment.

Purification of actinides using techniques such as ion-exchange, Solvent Extraction, Liquid membranes and Chromatographic Methods.

Hydrolysis, color, spectroscopy and magnetic properties of actinides, nuclear properties of actinides, decay modes.

#### ▪ Thorium

Isotopes, occurrence and production; Uranium: isotopes, occurrence, resources and production.

#### ▪ Trans uranium Elements

Production of transuranic elements, Neptunium, Plutonium, Americium and Curium; Actinide synthesis by heavy ion reactions. Fission Product Chemistry.

#### ▪ Aqueous Reprocessing

Introduction to nuclear fuel reprocessing; Need for reprocessing; PUREX, TRUEX, THOREX Latest developments. Solvent extraction for actinide purification; Basic principles, introduction to extractants, classification of extractants. Purification of uranium, plutonium; lanthanide actinide separations.

#### ▪ Pyro chemical Reprocessing

Introduction to non-aqueous reprocessing: Objectives and advantages of non-aqueous reprocessing in fast reactor fuel cycle, Advanced fuel cycle flow sheets involving non-aqueous reprocessing, Recent trends in pyrochemical reprocessing of oxide and metallic fuels.

Oxide electrowinning flow sheet, Pyrochemical reprocessing of metallic fuels (IFR process) - Integral Fast Reactor Concept, Differences in electrorefining and electrowinning.

NUMAC: Importance of Nuclear Material Accounting; techniques used for analysis of nuclear materials.

NUMAC with techniques such as Potentiometry, Coulometry, Amperometry.

Mass Spectrometry, Calorimetry, Gamma counting, neutron counting etc. Advantages and drawbacks of individual methods.

**Post Irradiation Techniques**

Introduction to post-irradiation examination methods of nuclear reactor fuels; importance of PIE methods, burn-up measurements; NDE testing of fresh fuel pins.

Non-destructive evaluation of irradiated fuels (X-ray and neutron radiographic examination of fuel pins, Fission gas analysis, Metallographic examinations).

**Nuclear Waste Management**

Introduction - industrial waste, nuclear waste & its speciality, generation of radioactive wastes, radioactivity in the environment, Solid, liquid

& gaseous wastes, international classification. Basic philosophy & methods of radioactive waste management, environmental monitoring. HLW & spent fuel waste. Radioactive waste immobilization matrices & their ultimate disposal.

**Course Outcomes:**

- Explore advanced chemical separations and purification techniques in nuclear fuel cycle.
- Evaluate chemical behavior of actinides and fission products in various media.
- Understand environmental and safety aspects of fuel cycle chemistry.
- Integrate chemical principles for efficient fuel recycling and waste minimization.

**References:**

1. G.T. Seaborg, In Handbook of Physics and Chemistry of Rare Earths: Lanthanides Actinides: Chemistry, Vol.18, (Eds., K.A. Schneider, Jr., L. Eyring, G.R. Choppin and G.H. Lander), Elsevier Science, Amsterdam (1994). Dynamic Mechanical Analysis: A Practical Introduction. K.P. Menars, CRC Press, Boca Raton, 1999. J.J. Katz, G.T. Seaborg and L.R. Morss, The Chemistry of Actinide Elements, Vol. 1 and 2, 2nd Ed., Chapman and Hall, New York (1986).
2. A.J. Freeman and C. Keller, Handbook of Physics and Chemistry of Actinides, North Holland Amsterdam, Vol.3 (1985), Vol.4 (1986), and Vol.6 (1991).
3. C. Keller, The Chemistry of Transuranium Elements, Verlag Chemie GmbH, Germany (1971).
4. G.T. Seaborg and D'E.Hobart, Summary of the Properties of Lanthanide and Actinide Elements' in 'Frontiers in Nuclear Chemistry', Eds. D.D. Sood, A.V.R. Reddy and P.K. Pujari, IANCAS publication, Mumbai (1996)
5. J.M. Cleveland, "The chemistry of plutonium" Gordon and Breach Science Publishers, New York, 1970.
6. Solvent Extraction of Metals, A. K. De, S. M. Khopkar and R. A. Chalmers, Van Nostrand, Reinhold (1970).
7. Ion Exchange and Solvent Extraction: A Series of Advances, Editors J. A. Marinsky and Y. Marcus, Marcel Dekker Inc. (1998).

## **CH11: Materials for Nuclear Reactors and Fuel Cycle Processing system (45L Hours) (02-CHEM04-609-C)**

**Coordinators: Dr. Rajesh Ganesan (rajesh@igcar.gov.in),  
Dr. Pushpalatha (pushpa@igcar.gov.in)**

### ***Course Details:***

- Coolants: Requirements, preparation, properties and handling. Water, liquid sodium, lead-bismuth alloys, helium, CO<sub>2</sub>.
- Coolant Chemistry: Na, Pb-Bi and Pb-Li chemistry: Monitoring and maintaining purity of coolants, on-line monitoring using EC monitors, sampling and analysis.
- Water chemistry: Fast reactor water chemistry, steam-water chemistry, condenser cooling and process water chemistry, de-mineralising plant and condensate polishing unit chemistry, on-line monitoring, biological shield cooling water chemistry, steam generator leak detection systems, related analytical techniques.
- Corrosion: Alkali metal corrosion.
- Moderators: Requirements, preparation, properties of H<sub>2</sub>O, D<sub>2</sub>O and graphite.
- Control Rod Materials: Requirements, preparation, enrichment, properties.
- Cover Gas: Cover gas purification, monitoring for hydrogen, fission gases.
- Decontamination: Sodium removal and decontamination of primary components of fast reactors, decontamination of thermal reactor primary components.

### ***Course Outcomes:***

- Examine materials used in reactor construction and fuel cycle facilities with focus on corrosion, radiation damage, and mechanical properties.
- Understand material degradation mechanisms under nuclear operating conditions.
- Develop strategies for material selection and life extension in nuclear systems.
- Analyze processing technologies relevant to nuclear materials handling and fabrication.

### **References:**

1. S. Glasstone, Source Book on Atomic Energy, Allied East-West Press Pvt. Ltd., New Delhi.
2. S. Glasstone and Sesonske, Nuclear Reactor Engineering, Chapman Hall, London, 1994.
3. H.U. Borgstedt and C.K. Mathews, Applied Chemistry of the Alkali Metals, Plenum Press, 1987.
4. C.C. Addison, The Chemistry of the Liquid Alkali Metals, John Wiley and Sons, 1984.
5. Power Plant Chemistry: A practical guide, Buecher Braid, Penwell, Oklahoma, 1997.
6. Modern Power Station Practice, III Edition, Pergamon, NY, 1992.

## CH12: Nuclear and Radiochemistry (45 Hours / 3 Credit) (02-CHEM04-612-C)

Coordinators: Dr. Sundararajan (sundar@igcar.gov.in),  
Dr. G V S Ashok Kumar (gvs@igcar.gov.in)

### Course Details:

- **Nuclear Properties**  
Concept of nucleus, nuclear spin, parity, electric and magnetic moments, isomerism, nuclear mass and binding energy, elemental abundance, radioactive decay laws, radioactive equilibria, Bateman's equation, liquid drop and shell models.
- **Nuclear Structure and Decay Modes**  
Nuclear force, structure of complex nuclei, liquid drop, shell and collective models, nucleon emission, beta decay, gamma de-excitation and internal conversion, selection rules.
- **Nuclear Reactions and Accelerators**  
Basic principles and energetics, cross sections, nuclear fission, charge and mass distribution in fission, compound nucleus reactions, direct reactions, types and details of accelerators.
- **Radiochemical Separations**  
Concepts of traces, chemical yields, radiochemical purity, applications.
- **Nuclear Techniques**  
Nuclear probes, PAC, NDA and on-line monitoring.
- **Radio-isotope Production**  
Basic principles of isotope production in both reactors and accelerators, Szilard - Chalmers effect and its utility, concept of generators, Molygenerators.
- **Applications of Radio-isotopes**  
Concepts of nuclear medicine and radio-pharmaceuticals, SPECT, PET, brachytherapy and teletherapy, Radio-immuno assay, industrial, agricultural and biological applications.
- **Laboratory Experiments**
  - Fission product separation and transient equilibrium.
  - Separation of actinides using ion-exchange or solvent extraction
  - Neutron activation analysis High resolution gamma spectrometry

**Course Outcomes:**

- Comprehend fundamental radioactive decay processes and nuclear reactions.
- Develop skills in radiochemical techniques and instrumentation.
- Understand applications of nuclear chemistry in medicine, industry, and research.
- Evaluate safety and regulatory frameworks governing radiochemical research.

**Reference:**

1. Nuclear and Radiochemistry (1981) - G. Friedlander, J. Kennedy, J.M. Miller and J.W. Macias
2. Atomic Nuclear (1955) - R.D. Evans
3. Source book of atomic energy (1969) - S. Glasstone
4. Essentials of Nuclear Chemistry (1982) - H.J. Arnikar.
5. The chemistry of Transuranium Elements (1971) - J. Keller
6. G.R. Chopin and Rydberg: Nuclear Chemistry, Theory and Applications, Pergamon Press, Great Transuranium elements and transactinides
7. Manual for reactor produced isotopes, IAEA-TECDOC-1340 (1999)
8. Radionuclides in therapy - R.P. Spencer, R.H. Sievers, A.M. Friedman. CRC Press (1987).
9. Radioimmunoassay: Principles and Practice, M.R.A. Pillai and S.D. Bhandarkar, 2nd Edition, BARC, 1998.
10. Industrial applications of radioisotopes - G. Foldiak

**CH13: Corrosion Science and Engineering (45L Hours) (02-CHEM04-613-C)**

**Coordinators: Dr. S Ningshen (ning@igcar.gov.in),  
Dr. C Jagadeeswara Rao (cjrao@igcar.gov.in)**

**Course Details:****▪ Thermodynamics of Aqueous Corrosion**

Electrode processes – electrode potential, free energy, EMF series, potential measurements with reference electrodes, three electrode systems, computation and construction of Pourbaix diagrams of Fe, Al, Ni and Zn, practical use of E-pH diagrams. Chemical Vs. electrochemical mechanisms of corrosion reactions, corrosion rate expressions.

**▪ Kinetics of Aqueous Corrosion**

Corrosion current density and corrosion rate, exchange current density. Polarization – activation control, Tafel equation, mass transport control, mixed potential theory and behavior of galvanic couples in acidic environments, effect of oxidizer, combined polarization, factors affecting polarizations and rate of corrosion. Passivity, potentiostatic polarization curves, factors affecting passivity, mechanism of action of passivators.

**▪ Forms of Corrosion**

General corrosion – atmospheric corrosion, galvanic corrosion, general biological corrosion. Localized corrosion – filiform corrosion, crevice corrosion, pitting corrosion, localized biological corrosion. Metallurgically influenced corrosion-inter granular corrosion, de-alloying. Mechanically assisted corrosion – erosion corrosion, fretting corrosion, corrosion fatigue. Environmentally induced cracking – mechanisms of stress corrosion cracking and hydrogen embrittlement.

**▪ Corrosion in Reactor and Reprocessing Plants**

Corrosion in liquid sodium, cooling water, sea water; Corrosion in nitric acid – effect of flow, environment and metallurgical variables of materials.

**▪ Prevention and Control of Corrosion**

Corrosion control by design. Selection of corrosion resistant materials – alloying, stainless steel and brass. Oxidation resistant materials, control of high temperature oxidation. Cathodic and anodic protection methods. Use of inhibitors-types. Corrosion in cold water pipes – Langalier saturation index.

**▪ Corrosion Monitoring**

Introduction – On-stream monitoring – Electrical resistance, linear polarization, hydrogen test probe, ultrasonic testing, radiography and corrosion coupons. Off-stream monitoring equipments – Acoustic emission testing, eddy current inspection, liquid penetration inspection.

**▪ Corrosion Testing**

Purpose and classification. Dimensional change – Ultrasonic thickness measurements, eddy current, microscopic examination. Weight change – Specimen preparation, test conditions and evaluation of results for overall corrosion, SCC, IGC. Electrochemical techniques – Polarization curves, Tafel extrapolation, linear polarization, AC impedance methods (EIS).

**Course Outcomes:**

- Understand the electrochemical basis and mechanisms of corrosion in metals and alloys.
- Analyze corrosion processes in nuclear reactor environments and fuel cycle components.
- Develop corrosion prevention and control strategies including coatings and material selection.
- Apply corrosion monitoring and testing techniques in industrial applications.

**Reference:**

1. Herbert H. Uhlig and R.Winston Revie, “Corrosion and corrosion control – An introduction to corrosion science and engineering”, Third Edition, John Wiley & Sons, 1985.
2. Mars G. Fontana, “Corrosion Engineering”, Third Edition, McGraw Hill Inc., 1987.
3. D.A.Jones, Principles and prevention of corrosion, Second Edition, Prentice Hall Inc, 1996.
4. ASM hand book – Vol 13: Corrosion, ASM International, 2001..
5. Philip A. Schweitzer, “Corrosion and corrosion protection handbook”, USA, 1983

## CH14: Quantum Chemistry & Group Theory (45L Hours) (02-CHEM04-614-C)

Coordinators: Dr. N Ramanathan (nram@igcar.gov.in),  
Dr. G Gopakumar (gopakumar@igcar.gov.in)

### Course Details:

#### ▪ **Fundamental of Principles**

Brief review of the fundamentals of quantum mechanics – postulates, measurements, operators, de Broglie equation, Heisenberg principle, Schrodinger Equation.

#### ▪ **Exactly solvable problems**

Particle in a box with walls at infinite and finite potential; Double box potential, tunneling, effect of barrier height on splitting of degenerate energy levels and its application in understanding double well potential. Particle in a ring. Simple harmonic oscillator, rigid rotor, hydrogen atom problem solution using both the power series method and ladder operators.

#### ▪ **Approximation Methods**

Variation method, perturbation theory for time-independent and time dependent systems; Many-electron systems: Hartree - Fock theory and beyond; Chemical binding in simple molecular systems: Valence bond and molecular orbital theories; Concept of LCAO and introduction to ab-initio and semi-empirical molecular orbital calculations of molecules

#### ▪ **Groups Theory**

Symmetry elements and operations, point groups, matrix representation, reducible and irreducible representations, the Great Orthogonality theorem, direct product representation, projection operators.

#### ▪ **Application of Groups Theory in Chemistry**

Vibrational problem, hybridization, SALC, ligand field theory.

### Course Outcomes:

- Understand quantum mechanical principles underlying atomic and molecular structure.
- Apply group theory to explain molecular symmetry and spectroscopic properties.
- Analyze chemical bonding and molecular orbitals through computational methods.
- Correlate advanced quantum chemistry concepts through variation and perturbation theorem with experimental observations in chemical systems.

### Reference:

1. "Quantum Chemistry", I. N. Levine, Allyn & Bacon, Inc. (Boston) 5ed. (2000).
2. "Introduction to Quantum Chemistry", F. S. Levine, Cambridge Univ. Press (2002).
3. "Quantum Chemistry", W. Kauzmann, Academic Press (1957).
4. "Chemical Applications of Group Theory", F. A. Cotton, Wiley Eastern Limited, (1989).
5. "Group Theoretical Techniques in Quantum Chemistry", C.D.H. Chisholm, Academic Press (1976).

## CH15: Quantum Chemistry & Group Theory (45L Hours) (02-CHEM04-614-C)

Coordinators: Dr. N Ramanathan (nram@igcar.gov.in),  
Dr. Satendra Kumar (sat@igcar.gov.in)

### Course Details:

- Vibrations and rotations of diatomic molecules, selection rules, nuclear spin statistics.
- Electronic spectroscopy of diatomic molecules, coupling of angular momentum, Hund's coupling cases, term states of molecules, potential energy functions - analytical and numerical (e.g. RKR), Dissociation energy, Franck Condon principle, numerical methods to evaluate Franck Condon factors.
- Vibrations of polyatomic molecules - classical mechanics of vibrations, symmetry and normal vibrations- applications of group theory.
- **Experimental techniques in spectroscopy**  
Fourier transform spectroscopy (FTIR, FT-RAMAN), time resolved FTIR and its applications in absorption and emission studies. Laser based experimental methods, Introduction and application of Terahertz spectroscopy.
- **Studies on ultrafast processes**  
Nanosecond and picosecond laser flash photolysis, fluorescence time domain spectroscopy with special emphasis on energy transfer and electron transfer reactions and studies on excited state properties.
- **NMR & ESR**  
Basics of NMR and ESR, Multipulse techniques in NMR, FTNMR, 2D-NMR. Time domain ESR, Electron Nuclear Double Resonance (ENDOR)-principle and applications.

### Course Outcomes:

- Understand principles behind atomic and molecular spectroscopic techniques such as microwave, IR, electronic (UV-VIS), NMR, and Raman
- Develop skills in interpreting spectroscopic data for molecular structure elucidation.
- Apply spectroscopic techniques to analyze chemical and nuclear materials.
- Utilize modern instrumentation and software tools for spectroscopic analysis.

### Reference

1. Modern Spectroscopy, J. M. Hollas, 4 Edn. John Wiley & Sons (2004)
2. Laser Spectroscopy: basic concepts and Instrumentation", W. Demtroder, Springer 2003, Berlin.
3. Introduction to Lasers Physics, K. Shimada, Springer Verlag, 1984 Berlin
4. Infra-Red spectra of Inorganic and coordination compounds, K. Nakamoto, 5 Ed, John Wiley 1978, New York.
5. Building scientific apparatus, John H Moore, Christopher C Davis and Michael A Coplan, 4th Edition, Cambridge University, 2009 Nuclear and Radiochemistry (3<sup>rd</sup> edition 2013) by G. Friedlander, J. Kennedy, J. M. Miller and J. W. Macias.
6. Fourier transform infrared spectroscopy, Peter R Griffiths & James A de Haseth, 2nd Edition, Wiley, 2007

**CH16: Lasers and Application (45L Hours) (02-CHEM04-616-C)**

**Coordinators: Dr Satendra (Kumarsat@igcar.gov.in),  
Dr Pavan Kumar Narayanam (pavankumarn@igcar.gov.in)**

**Course Details:**

- Rate equation for absorption, induced and spontaneous emission, Einstein's A and B coefficients – Concepts of laser action and population inversion – rate equations for two, three and four level systems.
- Laser and its sub-systems – Optical amplifier – optical resonator – excited state pump – Properties of laser beams – Spatial and temporal coherence.
- Different types of passive resonators, modes of a passive resonator – Active resonators – Gain & Threshold condition for lasing actions – laser modes – Gain saturation and mode competition – spatial and velocity hole burning.
- Wavelength and Intensity stabilization of lasers – turning of wavelength of lasers – prisms, grating and elations – controlled wavelength turning – Selection of axial modes, Experimental realization of single mode.
- Generation of short pulses – Q-switching and mode locking – active and passive methods.
- Principles of various types of lasers – UV, vis & IR lasers, metal vapour lasers, solid state lasers, Gas lasers, Dye lasers, Semiconductor-diode laser and free electron laser.
- **Laser Spectroscopic Techniques**  
Important features of lasers useful for spectroscopy – monochromaticity, directionality, high intensity, tunability, short pulses etc. Advantages of lasers for spectroscopy – high sensitivity and selectivity. Short review of spectral line broadening mechanisms.  
Doppler-limited spectroscopy
  - a) High sensitivity methods of Absorption – frequency modulation, intracavity absorption.
  - b) Photoacoustic spectroscopy;
  - c) Resonance ionization spectroscopy combined with mass spectrometry – multiphoton processes;
  - d) Optogalvanic spectroscopy
- **Laser Induced Fluorescence**
  - a) Molecular Spectroscopy by LIF;
  - b) Experimental aspects and advantages of LIF
  - c) LIF in supersonic molecular beams
- **Laser Raman Spectroscopy**
  - a) Linear Raman Spectroscopy;
  - b) Non-linear Raman Spectroscopy – Stimulated Raman scattering
  - c) Coherent Anti-Stokes Raman Spectroscopy (CARS)
- **Analytical applications of lasers**
  - a) Laser induced break down spectroscopy, cavity ring down spectroscopy;
  - b) Atmospheric measurements with LIDAR

▪ **Laser material interactions**

- a) Vaporization, desorption and ablation.
- b) Surface modification;
- c) Laser cooling
- d) Laser Induced Chemical Reactions/ Laser Isotope Separation

**Course Outcomes:**

- Understand physical principles of lasers and types of laser systems.
- Analyze laser-matter interactions relevant to spectroscopy, diagnostics, and materials processing.
- Develop knowledge of applications of lasers in chemical analysis and nuclear research.
- Gain practical skills in laser operation, safety, and experimental design.

**Reference**

1. Introduction to Lasers Physics”, K. Shimoda, Springer Verlag, 1984 Berlin
2. Laser Spectroscopy basic concepts and Instrumentation”, W. Demtroder, Springer 2003, Berlin.
3. Principles of lasers”, O. Svelto and D. C. Hanna, Plenum, 1989, New York
4. Chemical and biochemical applications of lasers-vol I & III”, C.B. Moore, (Ed) Academic Press, New York (1974)
5. Lasers”, P.W. Milonni and J.H. Eberly, World Scientific, Singapore (1981)

## CH17: Nanomaterials and Advanced Chemical Sensors (45 Hours / 3 Credit) (02-CHEM04-617-C)

Coordinators: Dr. Pavan Kumar Narayanam (pavankumarn@igcar.gov.in),  
Dr. A Sree Rama Murthy (asrm07@igcar.gov.in)

### Course Details:

#### ▪ Introduction

Nanoscale its importance, definitions, nanomaterial science-One dimension, Two dimensions(carbon nanotubes, inorganic nanotubes, nanowires, biopolymers), Three dimensions (nanoparticles, fullerenes C-60, dendrimers, quantum dots) properties (electrical, optical, mechanical & chemical).

#### ▪ Synthesis and characterization

Synthesis -Chemical methods (precipitation, sol-gel, CVD, ion- exchange, dispersion), Physical methods (milling, PVD, pyrolysis, ion-implantation). Consolidation of nanopowders – sintering introduction, theories of sintering, sintering of nanomaterials, novel methods for consolidation of Nano powders. Characterization – X-ray techniques, spectroscopic techniques, electron beam techniques, optical methods

#### ▪ Applications

Structural and functional ceramics, coatings, sensors, power sources, additives and catalysts, composites, lubricants, magnetic materials, medical implants & nuclear ceramics. Sintering – introduction, theories, methods for consolidation and sintering of nanostructured materials.

#### ▪ Introduction to chemical sensors

Fundamental definitions and principles; rationale of sensor design and operation; basic theoretical considerations.

#### ▪ Electrochemical sensors

(Potentiometric sensors, Voltammetric and Amperometric sensors)

Ion selective electrodes (ISEs) – principles, solid (glass and fast ion conductor based) and liquid membrane based electrodes Electrochemical gas sensors Semiconductor devices (ISFETs, MOSFETs) Conductance gas and vapour sensors based on metal oxides, semiconductors and conducting polymers. Biosensors- oxygen and glucose biosensors; mediated enzyme electrodes and enzyme field effect transistors (ENFETs).

#### ▪ Piezoelectric Sensors

Piezoelectricity and mechanical resonance: stress, strain and polarization; constitutive relationships; equations of wave motion and wave representation.

The transverse-shear mode sensor, or quartz crystal microbalance: application to gas- and liquid-phase sensing; applications to VOC sensing, immunosensing and biosensors.

#### ▪ Optical sensors

IR and UV sensors - semiconductors - optical irradiation – recombination - Quantum efficiency - p-n junctions - IV characteristics - forward bias and reverse bias - applications.

Micro Electro Mechanical System (MEMS) based sensors and electronic noses

Cantilever based sensors – Sensing Principles, types of cantilevers, use of different detection techniques, examples and applications

Chemo metrics as applied to chemical detection and identification; Olfaction and electronic noses; Salient features

▪ **Sensors fabrication methods**

Basics of Sensor configurations and geometries, Use of nano-materials in sensors Thin/thick film formation techniques (physical, chemical and LB film formation techniques), MEMs based sensor fabrication Surface analysis and characterization.

▪ **Practical**

- Testing of a solid electrolyte based potentiometric oxygen sensor
- Testing of an amperometric sensor for oxygen
- Fabrication and testing of a thick-film hydrogen sensor

**Course Outcomes:**

- Understand synthesis, characterization, and properties of nanomaterials.
- Analyze applications of nanomaterials in sensors and energy devices.
- Develop skills in designing and fabricating advanced chemical sensors with nanostructured materials.
- Evaluate the role of nanotechnology in enhancing sensor sensitivity, selectivity, and stability.

