

CHEMICAL SCIENCES

Programme Code: CHEM04

Programme Outcome:

- Basic concepts and fundamentals related to different sub-disciplines of chemistry
- Principles of synthesis, structure, coordination chemistry, structure -property relationships in various inorganic and bio-inorganic materials
- Understanding and application of concepts of theoretical and experimental chemistry to solving real world problems.
- Principles, concepts and application of different material characterization techniques
- Understanding the process of research formulation and design, methodology, data analysis using statistical tools and various ways of data presentation
- Understanding radioactivity, nuclear models, actinide chemistry and principles of different nuclear analytical techniques, reactors and accelerators.
- Knowledge of chemistry of nuclear fuel cycle from mining to waste management
- Production of radioisotopes and their societal applications
- Interaction of radiation with matter and its applications in detectors
- Materials, processes and technologies for energy conversion and storage
- Overview of structure, properties and applications of different kinds of inorganic materials with techniques to study them
- Fundamentals of different spectroscopic techniques and learning to interpret different spectra.
- Concepts, fundamentals and applications of computational chemistry
- Engagement in good research practices and life-long learning

DETAILED COURSE STRUCTURE

CORE COURSES				
Sr. No	Course Code	Subject Title	Hours (L)	Credits
1	CYJRF-107	Basic Inorganic Chemistry	15	1
2	CYJRF-108	Basic Physical Chemistry	15	1
3	CYJRF-109	Basic Organic Chemistry	15	1
4	CYJRF-110	Basic Analytical Chemistry	15	1
5	CYJRF-111	Basic Health Physics and Safety in Chemical Labs	15	1
6	CYJRF-112	Research Methodology	15	1
7	CYJRF-113	Research Publication and Ethics	30	2
Hours / Credits			120	8

ELECTIVE COURSES				
Sr. No	Course Code	Subject Title	Hours (L)	Credits
Group A (Any One)				
1	CYJRF-213	Nuclear & Radiochemistry	30	2
2	CYJRF-214	Chemistry Of Nuclear Fuel Cycle	30	2
3	CYJRF-215	Production And Applications of Radioisotopes	30	2
4	CYJRF-204	Radiation Detection and Measurement	30	2
5	CYJRF-207	Renewable Energy Harvesting and Storage	30	2
6	CYJRF-205	Advanced Material Chemistry	30	2
7	CYJRF-209	Advanced Spectroscopy	30	2
8	CYJRF-210	Computational Chemistry	30	2

SUMMARY				
Sr. No	Course	Quantity	Hours (T)	Credits
1	Core Courses	7 Nos.	120	8
2	Elective Courses	5 Nos.	150	10
Total Hours / Credits			270	18

CORE COURSES COORDINATOR

Chief Coordinators:

Dr. Vinita G. Gupta (ChD, Extn.: 22274, E-Mail: vinita@barc.gov.in)

Dr. Arunasis Bhattacharyya (RCD, Extn.: 26335, E-mail: arun12@barc.gov.in)

Course	Coordinators	Email ID
Basic Inorganic Chemistry	Dr. Dimple P. Dutta (HRDD)	dimpled@barc.gov.in
Basic Physical Chemistry	Dr. Manidipa Basu (ChD)	deepa@barc.gov.in
Basic Organic Chemistry	Dr. Dibakar Goswami (BOD)	deepa@barc.gov.in
Basic Analytical Chemistry	Dr. A.K. Satpati (ACD)	asatpati@barc.gov.in
Basic Health Physics & Safety in Chemical Labs.	Dr. P.S. Ramanjaneyulu (RACD)	psr@barc.gov.in
Research Methodology	Dr. Kallola Swain (ACD)	kallola@barc.gov.in
Research Publication and Ethics	Dr. Kallola Swain (ACD)	kallola@barc.gov.in

ELECTIVE COURSES COORDINATOR

Course	Coordinators	Email ID
Nuclear & Radiochemistry	Dr. B. Mahanty (RCD)	bmahanty@barc.gov.in
Chemistry of Nuclear Fuel Cycle	Dr. S.B. Deb (RACD)	sbdeb@barc.gov.in
Production and Applications of Radioisotopes	Dr. S. Chakraborty (RPhD)	sudipta@barc.gov.in
Radiation Detection and Measurement	Dr. Aishwarya Kar (RACD)	aishj@barc.gov.in
Renewable Energy Harvesting and Storage	Dr. Mrinal R. Pai (ChD)	mrinalr@barc.gov.in
Advanced Material Chemistry	Dr. Pramod Sharma (ChD)	pramod@barc.gov.in
Advanced Spectroscopy	Dr. S. Dutta Choudhury (RPCD)	sharmidc@barc.gov.in
Computational Chemistry	Dr. A. K. Pathak (ChD)	akpathak@barc.gov.in

CORE COURSES

CYJRF-107: Basic Inorganic Chemistry (15L Hours)

Coordinators: Dr. Dimple P. Dutta (HRDD)
dimpled@barc.gov.in

Course Details:

- **Co-ordination Chemistry**
Werner's Coordination theory, Valence Bond Theory, Crystal Field Theory, Jahn Teller effect, Thermodynamic effects of crystal field, Coordination chemistry of lanthanide and actinide ions, Application of group theory for d-d transition, Electronic spectra of complex ions, Absorption probability, Allowed transitions and selection rules, Tanabe Sugano diagram, Nephelauxetic effect, Ligand metal orbital overlaps, Magnetic properties of complex ions, f-f transitions in lanthanides. Molecular orbital theory, Molecular orbital diagram from concepts of group theory, MO's for Sigma bonding in AB₆ molecules, Tetrahedral AB₄ case, MO's for pi bonding in AB₆ molecules, Metal organic framework materials.
- **Solid state chemistry and crystallography (3 Hours)**
Crystalline and amorphous materials, Close packed structures, Lattice types and crystal systems, Basic structure types, Co-ordination number, Radius ratio rules, Silicate structures, Perovskites, Pyrochlores, Spinel, Structure of common nuclear materials. Fundamentals of X-ray crystallography, lattice, lattice planes, indices, crystal systems and symmetry. Diffraction of X-ray, Bragg's law, reciprocal lattice, structure factor, systematic absence, Different techniques of recording diffraction patterns.
- **Techniques for Synthesis of Materials (2 Hours)**
General concepts, Equipments/materials required with few typical examples, Scope and limitations of different synthesis techniques: Hydrothermal synthesis, Ultrasonication and Microwave synthesis, Metathesis, *chimiedouce* (polyol, co-precipitation, ion exchange), Gel combustion and sol-gel synthesis.
- **Magnetic, electrical and optical properties(4 hours)**
Behaviour of materials in magnetic field, Diamagnetic, Ferromagnetic, Anti-ferromagnetic, Paramagnetic materials with examples, Effect of temperature on magnetic materials, Application of magnetic materials. Band structures of metals, Insulators and semi-conductors, Controlled valency semiconductors, Dielectrics and concept of polarizability, Ferroelectrics, piezo and pyroelectric materials (concept, examples, applications), Phosphors, Photoluminescence, Electroluminescence, Thermoluminescence, Sensitizers, Activators, Excitation and emission spectra, Energy transfer, Defect-induced luminescence, Quantum yield, Application of phosphors.
- **Bioinorganic Chemistry (2 Hours)**
Metals in Biology: Nature's selection of elements in life, choice of redox active metal ions. Oxygen carrying proteins: hemoglobin and myoglobin, Reversible oxygen binding and transport. Introduction to medicinal inorganic chemistry, Platinum based anti-cancer drugs.

Course Outcomes:

- Understand principles of coordination chemistry, solid-state structures, and crystallography.
- Gain hands-on knowledge of synthesis and characterization of inorganic materials.
- Explore structure–property relationships in solids and coordination compounds.
- Appreciate the role of metals in biological systems through bioinorganic chemistry concepts.

Reference:

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.

CYJRF-108: Basic Physical Chemistry (15L Hours)

Coordinators: Dr. Manidipa Basu (ChD)
deepa@barc.gov.in

Course Details:

- **Thermodynamics**
Laws of thermodynamics, Concept of entropy, Fundamental equations and thermodynamic functions, Chemical potentials, Thermodynamics of solutions, ideal and regular solution models. Chemical Equilibrium: Partition function and equilibrium. Quantitative aspects of Faraday's laws of electrolysis, Nernst equation, Standard electrode (reduction) potential and its application to different kinds of half-cells. Degree of freedom rule .
- **Chemical Kinetics**
Rates of chemical reaction, rate equation, methods of determination of rate and order of a chemical reaction, complex reaction, Collision and transition state theories of chemical reaction, Potential energy surfaces and reaction dynamics. Application to unimolecular and Bimolecular reactions.
- **Quantum Chemistry**
Postulates of quantum mechanics, Classes of operator: Linear and Hermitian, Physical significance of eigen value in quantum mechanics; Boundary value problem in quantum mechanics; Exactly solvable problems: Particle in a box, rigid rotor and hydrogen atom; Approximation methods: Variation method; perturbation theory. 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.

Course Outcomes:

- Thermodynamic study helps in understanding energy transformations, and predicting system behavior, in general.
- Utility of kinetics study lies in understanding speed of chemical reactions and reaction mechanisms that are crucial in optimizing industrial processes and in predicting product yields.
- Quantum chemistry is useful for understanding molecular properties and reactions at molecular level which are essential for designing new materials.

References:

1. Fundamentals of Thermodynamics by Sonntag, R.E, Borgnakke, C & Van Wylen
2. Principles of Thermodynamics Hardcover by Jean-Philippe Ansermet, Sylvain D. Brechet
3. Chemical kinetics, by Keith J. Laidler
4. Atkins' Physical Chemistry by Julio de Paula and Peter Atkins
5. Quantum Chemistry by R. K. Prasad
6. Molecular Quantum Mechanics by Peter Atkins
7. Quantum Chemistry 7th Ed, Levine

CYJRF-109: Basic Organic Chemistry (15L Hours)

Coordinators: Dr. Dibakar Goswami (BOD)
dibakarg@barc.gov.in

Course Details:

- **Strategy and Design of Organic Synthesis**

Retro-synthesis analysis and synthetic-strategy, Enantio- and diastereo-selective synthesis, Solid phase synthesis, Concepts in combinatorial synthesis, Diversity oriented synthesis and their applications in various fields in chemistry including drug development, Catalysis and materials development.

- **Carbon-Carbon and C-X Bond Formation**

Various C-C and C-X coupling methods including single, double and triple bonds(Heck, Suzuki, Stille, Negishi, Kumada, Hiyama, Sonogashira, Buchwald-Hartwig reactions), Fischer and Schrock carbenes, Various types of metathesis reactions and application to organic synthesis, Organo-catalyzed organic reactions and enantio-selective organo-catalysis, C-H activation.

- **Organic Spectroscopy**

Organic absorption spectroscopy, examples of IR and UV spectra of simple organic molecules, Nuclear Magnetic Resonance spectroscopy (^1H and ^{13}C NMR spectroscopy), Fourier transform NMR, Mass Spectrometry, Interpretation of spectra and structural elucidation of organic molecules

Course Outcomes:

- Understand the concepts of designing the synthesis of various complex organic molecules.
- Understand various mechanisms prevailing in organic reactions.
- Basic understanding of organic spectroscopy techniques and structural elucidations.

Reference books:

1. Organic Chemistry by Jonathan Clayden, Nick Greeves and Stuart Warren
2. Organic Chemistry by Jerry March
3. Modern Physical Organic Chemistry by Eric V. Anslyn and Dennis A. Dougherty
4. Organic Spectroscopy by William Kemp
5. Organic Synthesis: The Disconnection Approach by Stuart Warren

CYJRF-110: Basic Analytical Chemistry (15L Hours)

Coordinators: **Dr. A.K. Satpati (ACD)**
asatpati@barc.gov.in

Course Details:

▪ Separation/Purification and Detection Technique

Solvent extraction: Conventional, Liquid membranes, Bulk, Supported and emulsified; Solid Phase Extraction (SPE); Ion Exchange: - Conventional, Membranes. Chromatography: -Gas Chromatography (GC), High Performance Liquid Chromatography (HPLC), Ion Chromatography (IC), Retention, Band spreading, resolution, Application of chromatographic techniques.

▪ Thermal Methods

Thermogravimetric Analysis (TGA); Derivative Thermogravimetric Analysis (DTG); Differential Thermal Analysis (DTA); Differential Scanning Calorimetry (DSC); Evolved Gas Analysis (EGA)

▪ Nuclear Methods

Neutron Activation Analysis (NAA); Charged Particle Activation Analysis (CPAA); X-ray fluorescence (XRF) spectrometry

▪ Electrochemical Methods

Potentiometry, Ion Selective Electrodes (ISE), Membrane ion selective electrodes, Voltammetry and Polarography, Cyclic, Pulse and Stripping Voltammetry, Electrochemical kinetics, Coulometry and Amperometry

▪ Spectrochemical Methods

Atomic Absorption Spectrometry:Flame (FAAS), Electrothermal (ETAAS), Cold Vapor (CVAAS), Hydride Generation (HGAAS); Optical Emission Spectrometry (OES): Inductively Coupled Plasma (ICPOES), Glow Discharge (GDOES).

▪ Mass Spectrometry

Mass Analysers: Magnetic, Quadrupole, Time of Flight (TOF), Ion Cyclotron Resonance; Detectors:- Faraday Cup, Channeltron, Daly; Ion Sources:- Thermal Ionization (TI), Electron Impact, ICP, GD, Laser Ablation (LA-ICP), Secondary Ionization (SI), Resonance Ionization (RI)

Course Outcomes:

- Learning the basics of analytical measurements using spectroscopy, electrochemistry, thermal, nuclear, separation and purifications techniques
- Understanding of Voltammetry in quantitative analysis, evaluation of redox and electrokinetic property of molecules and materials
- Utilization of nuclear techniques in nondestructive analysis, neutron activation analysis utilising nuclear reactor

Reference Books:

1. Encyclopaedia of Analytical Chemistry: Applications, Theory and Instrumentation, Editor R. A. Meyers, John Wiley & Sons Ltd. (2000).
2. Fundamentals of Analytical Chemistry, D.A. Skoog, D. M. West, F. J. Holler, S.R. Crouch, 8th Edition, Thomson (2004).
3. Principles of Instrumental Analysis, D.A. Skoog, F. J. Holler, T. A. Niemann, 5th Edition, Saunders College Publishing (1998).
4. A text book of Quantitative Analysis, A.I. Vogel, 5th Edition Revised by G. H. Jeffery, J. Bassett, J. Mendham and R. C. Denney, ELBS (1989).
5. Solvent Extraction of Metals, A. K. De, S. M. Khopkar and R. A. Chalmers, Van Nostrand, Reinhold (1970).

CYJRF-111: Basic Health Physics and Safety in Chemical Labs (15L Hours)

Coordinators: Dr. P.S. Ramanjaneyulu (RACD)
psr@barc.gov.in

Course Details:

▪ **Health Physics**

• **Fundamentals of Radiation Protection**

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

• **Basic Radiation Physics and Radiation Dosimetry Aspects**

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

• **Operational Monitoring and Safety Aspects of Facility Design**

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.

• **Radiological Safety Aspects in Design of Radio-Chemical Laboratories**

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

▪ **Safety in chemical labs**

Definition of chemical safety and its assessment, general chemical safety awareness, Classification of chemicals: Corrosive, Flammables, explosives, toxics, pyrophoric, carcinogen. Chemical which create lachrymation and smoke, Entry of such chemicals into human/biological system and its consequences, precautionary and safe methods for handling such chemicals, Compatibility issues

with chemicals, Understanding the Safety Data Sheets (Material Safety Data Sheets) for different chemicals. Storing different chemicals, incompatible chemicals, making inventory of chemicals, labelling chemicals depending upon its nature, safe disposal of chemicals, precautions and safe operating procedures (SOP) to be taken into consideration for chemical spills, chemical protective clothing, chemical accidents and their classification and consequences, Emergency Procedures during chemical accidents, Personal Protective equipment from chemical exposure, precautions to be taken with chemical which need to be refrigerated. Safe practices while using vacuum lines and laser. Fire safety and different types of fire extinguishers.

Course Outcomes:

- Understanding the fundamentals of radioactivity, the interaction of radiation with matter, and the principles of radiation detection.
- Understanding the basic principles of operational radiation protection.
- Understanding the basic concepts of safe operational procedures in chemical laboratories.

Reference:

1. Introduction to Health Physics by Herman Camber
2. International Commission on Radiological Protection (ICRP) Publication-103, 2007.
3. Biological Effects of Radiation by J. E. Coggle

CYJRF-112: Research Methodology (15L Hours)

Coordinators: Dr. Kallola Swain (ACD)
kallola@barc.gov.in

Course Details:

▪ **Objectives and Types of Research**

Motivation and objectives; Research methods vs. Methodology; Types of research: Descriptive vs. Analytical, Applied vs. Fundamental, Quantitative vs. Qualitative, Conceptual vs. Empirical; Stages of research; Research philosophy; Theory development; Research process.

▪ **Value of Statistics in Research**

Probability distributions: discrete and continuous; Normal distribution; Standard normal probability curve; Hypothesis testing: Definitions, basic concepts, procedure and flow diagram for hypothesis testing; Limitations of hypothesis testing; Important parametric tests.

Accuracy; Precision; Confidence interval, confidence limit and confidence level; Errors and Uncertainties: Classification of errors; Minimization of errors; propagation of errors; Tests for outliers; Limitation of analytical methods; Significant figures and rounding off rules; Reporting the results; Comparison of results: Z-test, students' t-test; F-test; Chi Square test for goodness of fit; Basic principles of analysis of variance; Setting up the ANOVA table, one way and two-way ANOVA; Use of statistical packages; Measure of asymmetries and other measures; Correlation and regression.

Determining experimental and sample designs; Measurement and scaling; Validity, reliability and practicality; Field work: The Nature of Field Work, Selection and Training of Investigators, Field Operation, Field Administration, Sampling frame and Sample selection.

Course Outcomes:

- Understand the concept of research methodology
- Importance of statistics in research
- Knowledge of various statistical tools used during research

Reference:

1. Garg, B.L., Karadia, R., Agarwal, F. and Agarwal, U.K., 2002. An introduction to Research Methodology, RBSA Publishers.
2. Kothari, C.R., 2000, Research Methodology: Methods and Techniques. New Age International.
3. Sinha, S.C. and Dhiman, A.K., 2002. Research Methodology, ESS Publications (2 volumes).
4. R. Paneer Selvam - Research Methodology Prentice Hall India Learning Private Limited; Second edition (2013)
5. Vogel's Text Book of Quantitative Inorganic Analysis, ELBS.
6. J.N. Miller, J.C. Miller, R.D. Miller, 2018, Statistics and chemo metrics for Analytical Chemistry, 7th Edition. Pearson Education Limited. UK.

CYJRF-113: Research Publication and Ethics (30L Hours)

Coordinators: Dr. Kallola Swain (ACD)
kallola@barc.gov.in

Course Details:

▪ **Research Formulation and Design**

Defining and formulating the research problem; Selecting the problem; Necessity of defining the problem; Importance of literature review in defining a problem; Literature review; Primary and secondary sources; reviews, treatise, monographs, patents, web as a source, searching the web; Critical literature review; Identifying gap areas from literature review; Development of working hypothesis, Research design; Basic Principles; Need of research design; Features of good design; Important concepts relating to research design; Observation and Facts; Laws and Theories, Prediction and explanation, Induction, Deduction; Development of Models; Collection of data through questionnaire and schedules; Collection of secondary data; Selection of appropriate method for collection, Guidelines for developing questionnaire; Successful interview; Survey v/s experiment; Developing a research plan - Exploration, Description, Diagnosis; Experimentation: Proper approach, Importance of recording observation, Maintaining the records, Sample history, Transparency in data recording.

▪ **Research Ethics**

Philosophy and ethics, Ethics with respect to Science and research, Intellectual honesty and research integrity, Application of results and ethics - Environmental impacts - Ethical issues - ethical committees - Commercialization - Scientific misconducts- fabrication, falsification, duplicate and overlapping publications, selective reporting and misrepresentation of data, Artificial Intelligence in Research Ethics.

▪ **Publication Ethics**

Definition, introduction and importance, Best practices, standards setting initiatives and guidelines, Conflict of interest, Publication misconduct, Violation of publication ethics, authorship and contributorship, Identification of publication misconduct, complaints and appeals, predatory journals and publishers. Plagiarism - Citation and acknowledgement - Reproduction of published material & and accountability.

Open Access Publications, Indexing Databases, Citation Databases: Web of Science, Scopus, Google Scholar etc. Impact Factor of Journals, CiteScore, h-index, i10 index etc.

▪ **Intellectual Property Rights (IPR)**

Intellectual property rights and patent law, Copy right - Royalty -Trade Related aspects of IPRs. Patent procedures in DAE.

▪ **Reporting and Thesis and Writing**

Structure and components of scientific reports - Types of report - Technical reports and thesis Significance - Different steps in the preparation - Layout, structure and Language of typical reports - Illustrations and tables - Bibliography, referencing and footnotes - Oral Presentation Planning - Preparation - Practice - Making presentation - Use of visual aids - Importance of effective communication -Computers in Chemistry, Usage of packages such as, Excel, AIM2000, ChemDraw, etc. Manuscript drafting based on 'Experimental data and Literature Survey'.

Course Outcomes:

- Familiarity with concepts of research formulations and design
- Understanding of ethical concepts during research and publications
- Better presentation of research outputs

Reference:

1. Anthony, M., Graziano, A.M. and Raulin, M.L., 2009. Research Methods: A Process of Inquiry, Allyn and Bacon.
2. Day, R.A., 1992. How to Write and Publish a Scientific Paper, Cambridge University Press.
3. David Resnick , 2005, The Ethics of Science, An Introduction, Taylor and Francis.
4. P. Chaddah, 2018, Ethics in competitive research: Do not get scooped; do not get plagiarized, ISBN: 978-9387480865.

ELECTIVE COURSES

CYJRF-213: Nuclear & Radiochemistry (30L Hours)

Coordinators: **Dr. B. Mahanty (RCD)**
bmahanty@barc.gov.in

Course Details:

- **Fundamentals of Radiochemistry**
 - **Radioactivity**
Nuclear stability, Binding energy, Natural radioactivity, Decay series, Induced radioactivity, Radioactive decay laws, Concept of half-life and radioactive equilibria
 - **Radioactive decay modes**
 α -decay, β decay, γ - deexcitation – basics
 - **Nuclear models**
Liquid drop model, Shell model, Basic concept of spin, parity electric and magnetic moments, Isomerism
 - **Artificial radioactivity**
Transmutation – concept of cross section, Energy thresholds, Fission and radioactivity formed in fission, Nuclear fusion, Basics of reactors and accelerators
 - **Radiotracers, dating and basic principles of nuclear analytical techniques**
- **Chemistry of Actinides**
 - **Basic Actinides Chemistry**
The Actinide Concept, Transuranium elements, Electronic configuration, Electronic states, Introduction to 'f' orbitals and their splitting in the ligand field. Relativistic effect and its consequences. Different spectroscopic techniques to understand the chemistry of Actinides (5h)
 - **Chemistry of Actinides in solution**
Ionic radii, Coordination number, Hydration Energy, Complexation with inorganic / organic ligands. Redox potentials, Eh-pH diagrams, Variable oxidation states, Ionic species, Hydrolysis, Polymerization / Depolymerization. (5h)
 - **Actinides in the environment**
Natural abundance of actinides, Oklo phenomenon, Actinide speciation in aquatic environment, Complexation with naturally occurring organics such as humic acid and fulvic acid, Sorption and Migration

Course Outcomes:

- Understanding the concept of radioactivity and the basics of different radioactive decay modes.
- Basic concepts on different nuclear models and artificial radioactivity.
- Understanding the principles of different nuclear analytical techniques, reactors and accelerators.
- Basic concept of actinide chemistry, f-orbital shapes, orbital splitting, redox potentials, Eh-pH diagram, speciation in aquatic medium

References:

1. Nuclear and Radiochemistry (1981) – G. Friedlander, J. Kennedy, J. M. Miller and J. W. Macias
2. Manmade elements (1963) – G. T. Seaborg
3. Essentials of Nuclear Chemistry (1982) – H. J. Arnikar
4. The Chemistry of Transuranium Elements (1971) – C. Keller
5. Fundamentals of Radiochemistry, IANCAS Publication, 2007.

CYJRF-214: Chemistry of Nuclear Fuel Cycle (30L Hours)

Coordinators: Dr. S.B. Deb (RACD)
sbdeb@barc.gov.in

Course Details:

- **Exploration, Mining, Milling & Processing of Uranium**
Occurrence & Minerals, Classification of U ore deposits, Exploration of U ore deposits, Mining and processing of U ore, Mill waste treatment, Development of U supported advanced fuel materials, U enrichment
- **Chemistry of Fuel Materials**
Separation and purification of uranium, thorium and zirconium from their ores, Principles and processes of isotope separation and enrichment of ^{235}U and deuterium, Conversion processes for preparation of UO_2 , $(\text{U,Pu})\text{O}_2$, $(\text{U,Th})\text{O}_2$, and advanced fuel materials like UC, $(\text{U,Pu})\text{C}$, UN $(\text{U,Pu})\text{N}$, metals and alloys. Thermophysical and thermochemical properties of nuclear fuel.
- **Nuclear Reactors and Related concepts**
Classification of reactors on the basis of neutron energy and reactor components, different reactor types like PHWR, BWR, PWR, AHWR, High Temperature Reactors, Molten salt reactor concept etc., Introduction of fusion reactor concept, Physico-chemical behaviour and properties of oxide, nitride and carbide fuels, Fuel fabrication processes & chemical quality control of fuel materials, Behaviour of nuclear fuels (thermal/fast) during irradiation, Post irradiation studies, fuel clad chemical interaction, Burn-up etc.
- **Chemistry of Back End of Nuclear Fuel Cycle**
Reprocessing of thermal reactor fuel using PUREX process, THOREX process, Reprocessing of fast reactor fuel, Classification of waste, Treatment practices of gaseous waste, low and intermediate level liquid waste, Partitioning of actinides from high level liquid waste, Mutual separation of lanthanides and actinides, separation of valuable isotopes, vitrification, immobilization matrices and transmutation. (5 Lectures)

Course Outcomes:

- Understanding the key stages of the nuclear fuel cycle.
- Explain the chemistry of fuel material preparation and fabrication.
- The reactor types and fuel behaviour under irradiation.
- Studying fuel reprocessing by PUREX and THOREX processes and waste management practices

References:

1. J.J. Kratz, G.T. Seaborg and L.R. Morss; The Chemistry of Actinide Elements, 2nd Edition, Vol. 1&2, Chapman & Hall, New York (1986).
2. J. J. Katz, L.R.Morss, J.Fuger, and N.M.Edelstein, Chemistry of Actinide and Transactinide Elements, 3rd edition, Springer, Berlin Volume 1-5, (2006).
3. J.C. Bailar, H.J. Emelius, R. Nyholm and A.F. Trotman-Dickenson; Comprehensive Inorganic Chemistry, Vol. 5, Pergamon Press, Oxford (1973).
4. A. J. Freeman and C. Keller (Eds.); Handbook of Chemistry and Physics of the Actinides, Vol. 1-6, North Holland Publishers, Amsterdam (1986).
5. G.R. Choppin and M.K. Khankhasayev; Chemical Separation Technologies and Related Methods of Nuclear, Waste Management, Kluwer Academic Publishers, Netherlands (1999).
6. B. S. Tomar, P. R. Vasudeva Rao, S. B. Roy, Jose P. Panakkal, Kanwar Raj, A. N. Nandakumar (Eds), Nuclear Fuel Cycle, Springer Nature, 2023.

CYJRF-215: Production and Application of Radioisotopes (30L Hours)

Coordinators: Dr. S. Chakraborty (RPhD)
sudipta@barc.gov.in

Course Details:

- **Production of Radioisotopes (8h)**

- **General Introduction and Decay Schemes of Some Important Radioisotopes**

Isotopes and radioisotopes, Naturally obtained and artificially produced radioisotopes, Need for radioisotope production, Basics of radioisotope production.

- **Production of Radioisotopes in a Nuclear Reactor**

Production of radioisotopes in a nuclear reactor - Various processes, Calculation of activity of radioisotope produced, 'No-carrier-added' and 'carrier-added' radioisotopes, Introduction to Szilard-Chalmer reaction and Bateman equation, Radiochemical processing of the irradiated targets - various techniques, Production routes and radiochemical processing for some important reactor radioisotopes: ^{60}Co , ^{99}Mo , ^{125}I , ^{131}I , ^{153}Sm , ^{192}Ir and ^{177}Lu .

- **Production of Radioisotopes in a Cyclotron**

Principles of production of radioisotopes in a cyclotron - Calculation of yield of radioisotopes produced in a cyclotron, Target preparation for production of radioisotopes in a cyclotron, Production and radiochemical separation of some important cyclotron produced radioisotopes: ^{18}F , ^{44}Sc , ^{64}Cu , ^{68}Ge , ^{89}Zr , ^{123}I , ^{124}I , ^{211}At and ^{225}Ac .

- **Radionuclide Generators**

Concept and applications of radionuclide generators, Separation methodologies used in generators, Calculation of elution yield and t_{max} , Examples of some clinically relevant radionuclide generator systems: $^{99}\text{Mo}/^{99\text{m}}\text{Tc}$, $^{68}\text{Ge}/^{68}\text{Ga}$, $^{90}\text{Sr}/^{90}\text{Y}$, $^{188}\text{W}/^{188}\text{Re}$, $^{225}\text{Ac}/^{213}\text{Bi}$ generators.

- **Applications of Radioisotopes & Radiation in Industry**

- **Radiotracer Applications**

Basic principle of radiotracer technology, Advantages of radiotracers, Selection of a radiotracer for a particular study, Injection and Detection of radiotracer, Radiotracer data treatment and analysis, Leak detection, Flow rate measurements, Residence time distribution measurements, Sediment transport investigations, Radiotracer applications in oil fields

- **Sealed Source Applications in Industry - Principle and Applications**

Radiometric measurements, Radiography, Nucleonic gauges.

- **Applications of Isotope Hydrology**

General principle of hydrology, Measurement techniques, Source and mechanism of recharge, Interconnection between water bodies, Determination of age of ground waters, Pollution studies.

- **Radiation Processing Applications**

Application of electron beam for processing of materials, Application of gamma radiations for processing of materials.

- **Applications of Radioisotopes & Radiation in Healthcare**
 - **Nuclear medicine and radiopharmaceuticals**
Nuclear medicine and its importance in human healthcare, Classification of radiopharmaceuticals, Characteristics of diagnostic and therapeutic radiopharmaceuticals, Mechanism of uptake of radiopharmaceuticals
 - **Preparation of radiopharmaceuticals**
Design and preparation of radiopharmaceuticals, Methods of radiolabeling, Radiolabeling with Technetium and Rhenium, Radiolabeling using novel cores such as Tricarbonyl, HYNIC, Nitride and '4+1' chemistry, Radiolabeling with Lanthanides, Gallium, Yttrium, Copper etc.,
 - **Quality control of radiopharmaceuticals**
Need for quality control of radiopharmaceuticals, Types of quality control tests, Physico-chemical quality control tests, Biological quality control tests
 - **Nuclear medicine imaging techniques**
Nuclear medicine imaging vs. other contemporary imaging techniques, Concept of tomography, Gamma camera, SPECT, PET and Hybrid imaging (SPECT-CT, PET-CT, SPECT-MRI, PET-MRI), SPECT vs. PET.
 - **Some important radiopharmaceuticals**
Some important organ-specific diagnostic (SPECT as well as PET radiopharmaceuticals) - Contemporary agents for Myocardial imaging, Brain imaging, Renal imaging, Hypoxia imaging, Tumor and inflammation imaging, Infection imaging, Receptor-specific imaging agents etc., Therapeutic radiopharmaceuticals for some specific applications - Bone pain palliation, Radiation synovectomy, Targeted radionuclide therapy, Peptide Receptor Radionuclidic Therapy (PRRT), Radioimmunotherapy (RIT), Targeted Alpha Therapy (TAT).
 - **Concept of theranostics and personalized medicine**
Concept of theranostics, Applications and advantages of theranostics in nuclear medicine, Theranostic radionuclides, Concept of personalized medicine.

Course Outcomes:

- Develop basic understanding of production of radioisotopes and their applications in healthcare, industry, agriculture, environment studies etc.
- Understanding the concept and procedure of production of radioisotopes suitable for various societal applications using nuclear reactors and accelerators
- Understanding of the application of radioisotopes in human healthcare, particularly as 'Radiopharmaceuticals'
- Detail understanding of how radioisotopes and radiation technology is used in industry

Reference:

1. Manual for Reactor Produced Isotopes. IAEA-TECDOC-1340, IAEA, 1999.
2. Dynamic Mechanical Analysis: A Practical Introduction. K.P. Menars, CRC Press, Boca Raton, 1999.
3. Industrial application of radioisotopes. G. Foldiak.
4. Guide Book on Radioisotope Tracers in Industry - Tech. Rep. Series 316, IAEA, Vienna, 1990.
5. Environmental Isotopes in Hydrogeology. Ian Clarke and Peter Fritz, Lewis Publishers, NY, 1997.
6. Fundamentals of Nuclear Pharmacy, G.B. Saha, Springer-Verlag, 1984.
7. Radiopharmaceuticals: Chemistry and Pharmacology, Adrian D. Nunn. Marcel Dekker, 1992.
8. Radionuclides in Therapy, R.P. Spencer, R.H. Sievers, A.M. Friedman. CRC Press, Boca Raton, 1987.
9. PET in Oncology: Basics and Clinical Applications, J. Ruhlmann, P. Oehr, H.J. Biersack. Springer-Verlag, 1998.
10. Fundamentals of Radiochemistry. D.D. Sood, A.V.R. Reddy, N. Ramamoorthy. Indian Association of Nuclear Chemists and Allied Scientists, 2004.

CYJRF-204: Radiation Detection and Measurements (30L Hours)

Coordinators: Dr. Aishwarya Kar (RACD)
aishj@barc.gov.in

Course Details:

- **Interaction of Radiation with Matter**
 - **Interaction of Heavy Charged Particle with matter**
Ionization in gaseous medium, Bragg curve, stopping power, Bethe Equation for stopping power, Range of heavy charged particles and straggling, Range energy relationship
 - **Interaction of Fast Electrons with Matter**
Comparison with heavy charged particle, LET for electron, Bremsstrahlung radiation, Bethe Equation, path length and range of electrons, Attenuation and absorption of β particles, Backscattering of β - particles
 - **Interaction of Electromagnetic Radiations (γ , X-Rays) with Matter**
Photoelectric Effect, Compton Scattering, Pair Production. Variation of cross section for different process with γ energy and Z of the medium, Attenuation and Absorption of gamma rays.
 - **Interaction of neutrons with matter**
Elastic and Inelastic Scattering of neutrons and slowing down, nuclear reactions
- **Radiation Detectors**
 - **Principle of Radiation Detectors**
Pulse height spectrum, Counting Characteristics, plateaus, Detection efficiency, Energy resolution, Dead time, Counting Statistics.
 - **Gas filled Detectors**
Ionization Chamber, Proportional counter, GM counter
 - **Scintillation Detectors**
Organic and Inorganic scintillators, Liquid scintillation counter, NaI(Tl) detector
 - **Semiconductor Detectors**
p-n junction, HPGe detector for gamma ray spectroscopy, Si(Li) for x-ray spectroscopy, Si surface barrier detector for alpha spectroscopy
 - **Neutron Detectors**
BF₃, ³He gas filled counters.
- **Solid State Nuclear Track Detectors (SSNTD)**
- **Instrumentation for nuclear techniques**
PMT and photo diodes, Single Channel Analyser, ADC, Multi ChannelAnalyser, basic coincidence circuit, determination of life time using coincidence system, Positron Annihilation Spectroscopy: Instrumentation and Applications, Perturbed angular correlation measurement: Instrumentation and Applications

Course Outcomes:

- Understand the fundamental interactions of ionizing radiation with matter.
- Understand the basic principles of radiation detectors and evaluate their performance suitability for specific applications.
- Understand nuclear instrumentation for radiation detection and advanced spectroscopy

References:

1. Radiation detection and measurement, G.F.Knoll, John Wiley & Sons

CYJRF-207: Renewable Energy Harvesting and Storage (30L Hours)

Coordinators: Dr. Mrinal R. Pai (ChD)
mrinalr@barc.gov.in

Course Details:

▪ **Basic Definitions and Classification**

Energy and development, Units, Dimensions and measurement systems, Conventional and non-Conventional Sources of energy, Energy from fossil fuels: Coal, Oil, Natural gas and Nuclear resources, Basics of Solar, Wind, Hydro, Tidal, Ocean thermal and Other renewable energy sources, Impact of energy on environment, Environmental pollution due to energy.

▪ **Energy Conversion Systems**

Basics of photovoltaic (PV) and PV systems, Thermochemical conversion through pyrolysis, Gasification and esterification, Bio-oil, Basics of hydrogen fuel, Fundamentals of fuel cells, Energy storage technologies, Chemical storage and electrical storage, Details of Pb-acid battery, Ni-Cd-alkaline battery.

▪ **Generation of Hydrogen**

Energy conversion and energy storage in photosynthetic organisms, Efficiency of photosynthesis, Thermochemical cycle for generation of hydrogen, Semiconductor materials, Metal oxide nano composites and their properties, Photochemical and Photoelectrochemical generation of hydrogen, Hydrogen storage materials.

▪ **Batteries, supercapacitors and Fuel Cells**

Cathode/anode materials, Electrolytes, Membranes, Chemical and Electrochemical processes in different batteries (Li ion, Na ion), Supercapacitors and fuel cells, Determination of fundamental parameters for characterization of the efficiency of batteries, Supercapacitors and fuel cells, Introduction to redox flow battery and different types of redox flow batteries, Hybridization of various energy storage systems such as battery-supercapacitors, Battery-fuel cell and Battery-supercapacitor, fuel cell for different applications.

Course Outcomes:

- Introduction to “Green hydrogen production and storage” relevant to the national green hydrogen mission
- (NGHM) of the country.
- Understanding of principles and materials for energy conversion processes
- Concepts, methods and materials for electrochemical energy storage

Reference Books:

1. Sustainable Energy without the hot air by David J. C. MacKay.
2. Solar energy engineering, Processes and systems, S. A. Kalogirou, 2nd Edition.
3. Solar Energy handbook, Michael Boxwell, 2017 Edition.
4. Photoelectrochemical Water Splitting: Materials, Processes and Architectures (Energy and Environment Series) 1st Edition, Hans-Joachim Lewerenz, Laurie Peter.
5. Advances in Photoelectrochemical Water Splitting: Theory, Experiment and Systems Analysis, Editors S David Tilley, Stephan Lany, Roel van de Krol.
6. Lithium ion batteries: Basics and applications, Editor R. Korthauer, Springer.
7. Supercapacitor: Instrumentation, Measurement and Performance Evaluation Techniques, Satyajit Ratha, Aneeya K. Samantara and, Springer.
8. Nanomaterials in Advanced Batteries and Supercapacitors, David J. Lockwood, Springer.

CYJRF-205: Advanced Materials Chemistry (30 Hours)**Coordinators: Dr. Pramod Sharma (ChD)**
pramod@barc.gov.in**Course Details:****▪ Nuclear materials**

Structure of common nuclear materials: Oxides (UO_2 , PuO_2 , ThO_2), metallic (U, Pu, Zr and its alloys, steel), carbides etc. Non-stoichiometry in nuclear materials and its significance, Concept of surrogates for nuclear materials, Materials relevant to back end of nuclear fuel cycle, Glasses and ceramics for waste immobilisation, Structure of components of SYNROC, Behavior of materials under irradiation (examples from front end and back end of nuclear cycle), dpa, Difference between effects of low and high energy irradiation.

▪ Carbon-based materials**• Classification**

Diamond, Graphite, graphite oxide, fullerenes, Carbon nano-tubes, Graphene, Glassy carbon, Diamond like carbon; Structural and thermodynamic basis of classification; Synthesis methods: Natural diamond, Synthetic diamond (HPHT and CVD methods), Graphite (natural and lab-made graphite, nuclear- grade graphite), fullerenes and CNT, Graphene synthesis; Properties: Physical and chemical properties (Structural-basis of origin of these properties), Unique properties of each carbon-form, Property-application correlation; Current applications and futuristic technological potential.

• Thermoelectric Materials:

Thermoelectric materials, Thomson, Peltier and Seebeck effects, Thermocouples, Hall effect, Materials used for thermoelectric energy conversion, Thermal conductivity and factors affecting it, Concepts of thermoelectric energy conversion, Figure of merit and factors governing it, Applications of thermoelectric materials

• Chemistry of Carbides, Borides, Nitrides

Synthesis, bonding, structure, properties and applications

▪ Materials Characterization Techniques**• Diffraction Techniques for Structural Analysis**

Brief description of diffraction techniques with some examples for indexing XRD patterns. Comparison of Powder and Single crystal X-ray diffraction, Neutron diffraction, Electron diffraction.

• Electron microscopic techniques

Electrons and their interactions with the specimen, Fundamentals of electron microscopy with emphasis on SEM and TEM, Overview of the instruments, Magnetic lenses and deflectors, Electron guns, Lens aberrations and basic operation modes: Bright field and dark field imaging, Diffraction modes, Different electron microscopy techniques and applications, Image analysis using SEM and TEM, Introduction to advanced microscopic techniques: EDX,

HAADF-STEM, EELS, electron tomography etc.

- **Advanced Techniques for Materials Characterization**

Different characterization techniques based on X-rays and electrons: XRF, EPMA, XPS, AES, EELS, EXAFS and their application with examples, Concept and examples of Characterization Techniques based on Nuclear Reactions and Ion Beams: Rutherford Back Scattering Spectrometry (RBS), Elastic Recoil Detection Analysis (ERDA), Nuclear Reaction Analysis (NRA), Particle Induced X-ray Emission (PIXE) and Particle Induced Gamma-ray Emission (PIGE), Techniques employing Nuclear Probes: Positron annihilation spectroscopy (PAS): Lifetime spectroscopy, Doppler broadening spectroscopy, Age momentum correlation, Applications with examples, Perturbed angular correlation (PAC) techniques and their applications with examples.

Course Outcomes:

- Understanding principle and application of different characterization techniques
- Knowledge of synthesis, structure, properties and application of non-oxide materials
- Overview of structure and properties of oxides and non-oxide materials with nuclear relevance

Reference Books:

1. Solid State Chemistry and its Applications by A. R. West
2. Material Science and Engineering by V. Raghavan
3. New Directions in Solid State Chemistry by C. N. Rao and J. Gopalakrishnan
4. Solid State Chemistry: An Introduction by Smart and Moore
5. Introduction to Solid State Physics by Charles Kittel

CYJRF-209: Advanced Spectroscopy (30L Hours)**Coordinators: S. Dutta Choudhury (RPCD)**
sharmidc@barc.gov.in**Course Details:****▪ Vibrational Spectroscopy****• Infra-Red Spectroscopy**

Harmonic oscillator and the rigid rotator spectroscopic model, Harmonic oscillator (Hooke's Law), Hermite polynomials, Anharmonic oscillator, Selection rules, Rigid rotator, Rotating diatomic model, Vibrating diatomic molecule, Diatomic vibrating rotator, Vibro-Rotational spectrum for simple molecules, Born- Oppenheimer approximation (BOA), Vibrations of polyatomic molecules, Symmetry of molecules and vibrational spectroscopy, Influence of rotation on polyatomic spectra, Techniques and instrumentation for FT- IR, Analysis of functional groups by IR, 2D-IR.

• Raman Spectroscopy

Basic concept of Raman Spectroscopy, Quantum mechanical model of Raman scattering, Rayleigh scattering, Stokes and anti-Stokes scattering, Polarizability of the molecules, Selection rules for rotational Raman spectra of diatomic molecules, Rotational Raman spectra, Vibrational Raman spectra, Raman spectra of polyatomic molecules, FT-Raman, Instrumentation and techniques, Enhanced Raman Spectroscopy (SERS, TERS).

▪ Spin Spectroscopies**• Nuclear Magnetic Resonance (NMR)**

Nuclei with intrinsic spin Angular momentum, Magnetic moments interaction with magnetic fields, P- NMR, (n+1) rule, First order spectra, Spin-spin coupling, Multiplets in NMR spectroscopy, Spin-Spin Coupling between chemically equivalent, Second order spectra and vibrational method, Nuclear Overhauser Effect, C13-NMR, 2D and Correlated 2D NMR spectroscopy, Chemical Shift Anisotropy (MAS-NMR), Solid state NMR- Si29-NMR, F19NMR etc.

• Electron Paramagnetic Resonance (EPR)

A brief review of theory, Analysis of ESR spectra of systems in liquid phase, Radicals containing single set, Multiple sets of protons, Triplet ground states, Transition metal ions, Rare earth ions, Ion in solid state, Double resonance techniques: ENDOR in liquid solution, ENDOR in powders and non-oriented solids.

• Mossbauer Spectroscopy

Basic physical concepts, Spectral line shape, Isomer shift, Quadrupole splitting, Magnetic hyperfine interaction, Interpretation of Mossbauer parameters of ⁵⁷Fe, ⁹⁹Ru, ¹⁰¹Ru, ¹⁹⁵Pt, ¹⁹³Ir and ¹¹⁰Sn, General applications of Mossbauer like - Solid state reactions, Thermal decomposition, Ligand exchange, Electron transfer, Isomerism, Surface studies and biological applications etc.

- **Photo Electron Spectroscopy**

XPS, AES and UPS: Background to electron beam techniques, XPS and AES processes, UHV conditions, X-Ray Sources, Electron Sources, Ion Sources, Spectral Interpretation, Nomenclature (j-j & L-S coupling), Elemental detection, Electron-excited secondary electron spectrum-AES, XPS-Primary, Secondary Structure, Angular effects, Time dependent spectra, Depth profiling, Data analysis: Curve fitting, Co-ordination number, Surface states, Ultraviolet Photoelectron Spectroscopy (UPS).

- **Electronic Spectroscopy**

Intensity of electronic transitions, Rules governing the transition between two states, Excited electronic states of atoms and molecules, Types of electronic transitions in organic molecules, Potential energy diagrams, Absorption band and Frank-Condon Principle, Emission spectra, Excited state-dipole moment, Photo physical pathways, Internal conversion and Interstate crossing, Emission property, Fluorescence, Phosphorescence, Photoluminescence Spectroscopy, UV-Vis spectra for solids, Band gap determination, Kubelka- Munk theorem.

Course Outcomes:

- Overview of photoelectronic, electronic, vibrational and spin spectroscopies.
- Understand the transition mechanisms, experimental techniques and instrumentation involved in each case.
- Interpretation of spectra for applications in various fields

Reference:

1. Organic Spectroscopy. William Kemp. McMillan Publications.
2. Spectrometric Identification of Organic Compounds. Francis X. Webster, Robert M. Silverstein. Wiley Publications.
3. Fundamentals of Molecular Spectroscopy. CN Banwell EB Mccash.
4. Physical Chemistry: A Molecular Approach. Donald A. McQuarrie. John D. Simon.

CYJRF-210: Computational Chemistry (30L Hours)

Coordinators: Dr. A. K. Pathak (ChD)
akpathak@barc.gov.in

Course Details:

- **Electronic Structure Theory of Molecules**

Introduction, Revision to classical mechanics and quantum mechanics, Optimization techniques, Electronic structure methods: Self Consistent Field Theory, Restricted & unrestricted HF, Semi-empirical methods, Electron correlation methods: Configuration interaction Methods, Multi Configuration Self-Consistent Field, Many body perturbation theory, Couple cluster method, Basis sets, Density functional methods, Wave functional analysis & Molecular properties

- **Theory of Solids**

Geometry of crystal and symmetries in solids, Concept of reciprocal space and its use in solid state research and band structure, Introduction of energy bands in solids & Density of States, Determination of band structure (Kronig-Penny Model- analytical solution), Comparison of band structures (Metal (bcc, fcc, hcp), Insulators and Semi-conductors)

- **Multi-scale material modelling (MMM)**

Overview, Different length scales and associated timescales relevant to different computational methods, Atomistic modeling of materials: Why computer simulation of a many-body system at finite temperature, Born Oppenheimer (BO) approximation and the origin of different Molecular Dynamics (MD) methods such as B.O. MD, CPMD and classical MD.

- **Interatomic Potentials**

Introduction to interatomic potentials, expressing many-body potentials into suitable tractable form, Simplification due to homogeneous, isotropic approximation, Characteristics of potential, Obtaining potential function for a particular system, Different forms of Empirical potential functions such as Hard Sphere Potential, Lennard-Jones Potential, Morse Potential etc., Many-body potentials such as Embedded Atom Potential, Glue potential etc.

- **Molecular Dynamics Simulations**

An algorithm, Initialization, Boundary Conditions: Periodic Boundary Condition and Minimum Image Condition, Force Calculation & force subroutine, Integrating the Equations of Motion: Verlet, Velocity-Verlet & Leap Frog Algorithm

- **Statistical Mechanics and Molecular Dynamics simulation**

Multi-dimensional phase-space and time averaging, Ensemble and Ensemble averaging, Ergodicity and the equivalence of time and ensemble averages, Judging Equilibration

- **Application of Statistical Mechanics to get different average equilibrium properties from the microscopic quantities of the simulation**

How to get different equilibrium properties, Temperature and Pressure, Radial Distribution functions and structure factor, Time Correlation function and different dynamical quantities from equilibrium simulations, How to calculate Diffusivity, Thermal conductivity, electrical conductivity, viscosity etc

Course Outcomes:

- Provide the knowledge of electronic structure calculations of molecules to materials and molecular dynamic simulations of large systems.
- Developing the concept of computational chemistry for practical applications.
- Helps with how to handle problems of all lengths (atom to bulk) and time scales (fm to years).

Reference

1. An Introduction to computational chemistry by Frank Jensen (Wiley)
2. Quantum chemistry by I R Levine
3. Solid State Physics by M A Wahab
4. Computer simulation of liquids by Allen & Tildesley
5. Advanced Techniques for Materials Characterization"; Eds. A. K. Tyagi, M. Roy, S. K. Kulshreshta, S. Banerjee; Trans Tech Publications Ltd, Switzerland (2009)
6. Nuclear and Radiochemistry (3rd edition 2013) by G. Friedlander, J. Kennedy, J. M. Miller and J. W. Macias.
7. Ion Beam Analysis: Fundamentals and applications by Michael Nastasi, James W. Mayer, Yongqiang Wang.
8. Physical Principles of Electron Microscopy: An Introduction to TEM, SEM, and AEM, Springer, 1st ed. 2005
9. R. Haynes, Optical Microscopy of Materials, Springer, 1984