PG & RESEARCH DEPARTMENT OF PHYSICS

NATIONAL COLLEGE
(AUTONOMOUS)

TIRUCHIRAPPALLI

M. Phil.- SYLLABUS

FROM JUNE 2019 ONWARDS

M.Phil. PHYSICS (For the candidates admitted from the year 2019 - 20 onwards)

CORE COURSE –I
RESEARCH METHODOLOGY AND NUMERICAL METHODS

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Understand the basic Ideas of Research
CO2: Explain the ideas of Modern Research practice in scientific research
CO3: Bring out the elementary ideas about Data Analysis
CO4: Explain the methods of Data analysis by various statistical methods
CO5: Understand about Numerical Differentiation and iterative methods suitable for research

UNIT- I: BASICS OF RESEARCH

Meaning, purpose and characteristics of research – Characteristics of a researcher- Classification of research- Research process- Scientific research – Aim and motivation- Principles and ethics - Identification of research problem-Formulation of objectives execution plan – Current status – Literature survey – Abstraction of a research paper – Access using internet web tools – e-mail – Impact and usefulness of the research problem – Role of research guide – Guidance and rapport - Preparation and presentation of scientific reports- Need and methods (Oral and poster) –Writing of synopsis and dissertation and thesis.

UNIT- II: MODERN RESEARCH PRACTICES IN SCIENTIFIC RESEARCH

Usage of open source software and freely licensed software for research work and data analysis – Effective use of internet for research needs-Collaborative work-Interdisciplinary research-Scholarly research articles – National, International and Electronic journals - Online submission of research articles -Open access articles-benefits- Impact factor, h-index- Citations- ISBN- ISSN, Seminars, workshops, conferences and symposia- Respecting copy rights- Avoiding plagiarism- Intellectual property rights and patents.

UNIT -III: DATA ANALYSIS

Approximate numbers and Significant figures – Rounding of Numbers – Absolute, Relative and Percentage errors – Relation between relative error and the significant figures – The general formula for errors – Formulas to the fundamental operations of arithmetic and logarithms – Accuracy in the evaluation of a formula – Accuracy in the determination of arguments from a tabulated function – Accuracy of series approximations.

UNIT- IV: METHODS OF DATA ANALYSIS

Data-data collection – Statistical description of data (mean, variance, skewness, median, and mode) – Distributions (Student's t-test, F-test, Chi-square test), Correlation (linear and nonparametric/rank); Modeling data: Least squares, fitting data – Linear and non-linear models. Pictorial representation of data – Use of open source statistical software packages for computational needs (basic ideas).

UNIT- V: NUMERICAL METHODS

Numerical solution of Ordinary Differential Equations: Single step methods: Picard's method, Runge - Kutta II order and IV order methods. Multi step methods: Predictor – Corrector method: Milne and Adam-Bashforth methods.

Iterative methods for Eigen values: Power method, Jacobi method (up to 3x3 matrices and problems only).

BOOKS FOR STUDY AND REFERENCES:

1. G. Vijayalakshmi and C. Sivapragasam, Research Methods (Tips and techniques) MJP publishers, Chennai (2008).
2. K. Ravichandran, K. Swaminathan, B. Sakthivel, A.T. Ravichandran, Research Methodology and Scientific Writing: Jazym Publications (2017).
3. Lecture notes and course material: Modern Research Practices in Scientific Research by Dr.T.V.Sundar, Department of Physics, National College (Autonomous), Tiruchirappalli (2018).
4. Internet: An Introduction, CI Systems School of Computing, Jaipur, Tata Mc Graw Hill, New Delhi (1999).
5. Gupta.S.C & Kapoor.V.K, Fundamentals of Mathematical Statistics, Sultan Chand & sons, New Delhi (1994).
6. M.K. Jain, S.R.K. Iyengar and R.K. Jain, Numerical Methods for Scientific and Engineering Computation, New Age International Private Limited (1999).
7. P. Kandasamy, K. Thilagavathy, K. Gunavathi, Numerical Methods, S Chand & Co. Ltd.(2006).

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CORE COURSE– II: ADVANCED PHYSICS

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Understand the ideas about techniques of crystal growth and thin films
CO2: Explain about nanotechnology and types of nano structures
CO3: Bring out the elementary ideas about electron microscopy
CO4: Explain the various spectroscopic techniques
CO5: Understand about X-ray diffraction and types of diffractometers.

UNIT- I: CRYSTAL GROWTH TECHNIQUES AND THIN FILM PHYSICS

Crystal Growth Techniques: Nucleation-Spherical and cylindrical nucleation-Solution growth methods: Slow cooling, slow evaporation, Melt growth: Bridgeman method-Czochralski method.

Thin film physics: Physical methods-Thermal evaporation-Electron beam evaporation-Sputtering method-Spray pyrolysis-Chemical Vapour Deposition (CVD).

UNIT -II: NANOTECHNOLOGY

Nanotechnology: Importance of Nano materials- Types of nano structures (1D, 2D, 0D) - Self Assembled Monolayers (SAM)-Vapour Liquid Solid (VLS) - Carbon Nano Tubes (CNT)-Metals (Ag, Au) - Metal oxides (TiO_2, ZnO)-Semiconductors (CdS, ZnSe).

UNIT- III: ELECTRON MICROSCOPY

SEM, EDAX, and TEM: Working principle and Instrumentation – Sample preparation – Data collection, processing and analysis- Scanning Tunneling Microscopy (STEM).

UNIT -IV: SPECTROSCOPIC TECHNIQUES

Principles and instrumentation for UV-Vis-IR, FTIR spectroscopy, ESR, NMR, XPS– Rutherford Back Scattering (RBS) analysis - Applications. X-ray fluorescence spectroscopy –Advantages and its applications.

UNIT- V: X-RAY DIFFRACTION METHODS

Powder diffraction - Powder diffractormeter - Interpretation of diffraction patterns - Indexing - Phase identification - Residual stress analysis - Particle size, texture studies. Single crystal X-ray Diffractometer - Construction, working and uses.

REFERENCES:

1. J.C.Brice, Crystal Growth Processes, John Wiley and sons, New York (1986).
2. P.Santhana Raghavan and P.Ramasamy, Crystal Growth Processes and Methods, KRU Publications, Kumbakonam (2000).
3. A.Goswami, Thin Film Fundamental, New Age International (P) Ltd. New Delhi (2006).
4. Leonard C.Feldmann and James W.Mayer, Fundamentals of Surface and Thin Film Analysis.
5. G.Cao, Nano Structures and Nano materials: Synthesis properties and applications, Imperical College press (2004).
6. K.Ravichandran, K.Swaminathan, B.Sakthivel, A.T.Ravichandran, 'Introduction to Thin Films': Jazym Publications (2017).
7. Stradling. R.A; Klipstain. P.C; Growth and Characterization of semiconductors, Adam Hilger, Bristol (1990).
8. Belk. J.A, Electron Microscopy and Microanalysis of Crystalline Materials, Applied Science Publishers, London (1979).
9. Lawrence E. Murr, Electron and Ion Microscopy and Microanalysis Principles and Applications, Marcel Dekker Inc., New York (1991).
10. D. Kealey and P.J. Haines, Analytical Chemistry, Viva Books Private Limited, New Delhi (2002).
11. Instrumental Methods of Chemical Analysis, B. K. Sharma, GOEL Publishing House (2001).
12. Elementary Crystallography, D. Velmurugan, MJP Publishers, Chennai (2008).

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COURSE– III: TEACHING AND LEARNING SKILLS

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Acquaint different parts of computer system and their functions.
CO2:Develop skills of ICT and apply them in teaching learning context and research.
CO3: Appreciate the role of ICT in teaching, learning and Research.
CO4:Understand the terms communication technology and computer mediated teaching and develop multimedia /e- content in their respective subject.
CO5:Develop different teaching skills for putting the content across to targeted audience.

UNIT- I: COMPUTER APPLICATION SKILLS

Information and Communication Technology (ICT): Definition, Meaning, Features, Trends – Integration of ICT in teaching and learning – ICT applications: using word processors, spread sheets, power point slides in the classroom – ICT for Research: On-line journals, e-books, courseware, tutorials, technical reports, theses and dissertations.

ICT FOR PROFESSIONAL DEVELOPMENT

Concept of professional development- Institutional efforts for competency building- Individual learning for professional development using professional networks, OERs, technology for action research, etc.

UNIT- II: COMMUNICATIONS SKILLS

Communication: Definitions – Elements of communication: sender, message, channel, receiver, feedback and noise – Types of communication: spoken and written; non-verbal communication – Intrapersonal, interpersonal, group and mass communication – Barriers to communication: mechanical, physical, linguistic and cultural – Skills of communication: listening, speaking, reading and writing – Methods of developing fluency in oral and written communication – Style, diction and vocabulary – Classroom communication and dynamics.

UNIT- III: PEDAGOGY

Instructional Technology: Definition, objectives and types – Difference between teaching and instruction – Lecture technique: steps, planning of a lecture, delivery of a lecture – Narration in tune with the nature of different disciplines – Lecture with power point presentation - Versatility of lecture technique – Demonstration: characteristics, principles, planning implementation and evaluation – Teaching-Learning techniques: Team teaching, group discussion, seminar, workshop, symposium and panel discussion.

UNIT- IV: e- LEARNING, TECHNOLOGY INTEGRATION AND ACADEMIC RESOURCES IN INDIA

Concept and types of e-learning (synchronous and asynchronous instructional delivery and means), m-learning (mobile apps); blended learning; flipped learning; e-learning tools (like LMS; software's for word processing, making presentations, online editing, etc.); subject specific tools for e-learning; awareness of e-learning standards- Concept of technology integration in teaching- learning processes; frameworks guiding technology integration (like TPACK; SAMR); Technology Integration Matrix- Academic resources in India: MOOC, NMEICT; NPTEL; e-pathshala; SWAYAM, SWAYAM Prabha, National Academic Depository, National Digital Library; e-Sodh Sindhu; virtual labs; e-Yantra, Talk to a teacher, MOODLE, mobile apps, etc.

UNIT- V: SKILLS OF TEACHING AND TECHNOLOGY BASED ASSESSMENT

Teaching skills: Definition, Meaning and Nature- Types of teaching skills: Skill of set induction, skill of stimulus variation, skill of explaining, skill of probing questions, skill of black board writing and skill of closure – Integration of teaching skills – Evaluation of teaching skills.

Technology for Assessment: Concept of assessment and paradigm shift in assessment; role of technology in assessment 'for' learning; tools for self & peer assessment (recording devices; e-rubrics, etc.); online assessment (open source software's; e-portfolio; quiz makers; e- rubrics; survey tools); technology for assessment of collaborative learning like blogs, discussion forums; learning analytics.

REFERENCES

1. Bela Rani Sharma, Curriculum Reforms and Teaching Methods, Sarup and sons, New Delhi (2007).
2. Brandon Hall , e-learning, A research note by Namahn, found in: www.namahn.com/resources/ .../note-e-learning.pdf, Retrieved on 05/08/2011
3. Don Skinner, Teacher Training, Edinburgh University Press Ltd., Edinburgh (2005).
4. Information and Communication Technology in Education: A Curriculum for schools and programmed of Teacher Development, Jonathan Anderson and Tom Van Weart, UNESCO (2002).
5. Jereb. E. & Šmitek. B., Applying multimedia instruction in e-learning. Innovations in Education and Teaching International, 43(1), 15-27(2006).
6. Kumar, K.L, Educational Technology, New Age International Publishers, New Delhi (2008).
7. Learning Management system: https://en.wikipedia.org/wiki/Learning_management_system, Retrieved on 05/01/2016
8. Mangal. S.K, Essential of Teaching – Learning and Information Technology, Tandon Publications, Ludhiana (2002).
9. Michael.D and William, Integrating Technology into Teaching and Learning: Concepts and Applications, Prentice Hall, New York (2000).
10. Pandey.S.K, Teaching communication, Commonwealth Publishers, New Delhi (2005).
11. Ram Babu. A and Dandapani. S, Microteaching (Vol.1 & 2), Neelkamal Publications, Hyderabad (2006).
12. Singh.V.K and Sudarshan K.N., Computer Education, Discovery Publishing Company, New York (1996).
13. Sharma. R.A., Fundamentals of Educational Technology, Surya Publications, Meerut (2006).
14. Vanaja.M and Rajasekar.S, Computer Education, Neelkamal Publications, Hyderabad (2006).

Course Outcomes

After completing the course, the students will:

1. Develop skills of ICT and apply them in Teaching Learning context and Research.
2. Be able to use ICT for their professional development.
3. Leverage OERs for their teaching and research.
4. Appreciate the role of ICT in teaching, learning and Research.
5. Develop communication skills with special reference to listening, speaking, reading and writing.
6. Learn how to use instructional technology effectively in a classroom.
7. Master the preparation and implementation of teaching techniques.
8. Develop adequate skills and competencies to organize seminar / conference / workshop / symposium / panel discussion.
9. Develop skills in e-learning and technology integration.
10. Have the ability to utilize academic resources in India for their teaching.
11. Have the mastery over communication process through the web.
12. Develop different teaching skills for putting the content across to targeted audience.
13. Have the ability to use technology for assessment in a class room.

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ELECTIVE COURSE– IV: MATERIALS SCIENCE

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Study the crystal structure
CO2: Study nucleation and kinetics of crystal growth
CO3: Learn solution growth techniques
CO4: Learn melt and vapour growth techniques
CO5: Study the analytical techniques

UNIT - I: CRYSTAL STRUCTURE

Periodic array of atoms -Symmetry operations- The basis and crystal structure-Primitive cell- Fundamental types of lattices-Simple crystal structures- Crystal diffraction and reciprocal lattices-Experimental diffraction methods-Diffraction types-Bonding in solids and their characteristics.

UNIT - II: NUCLEATION

Nucleation – Theories of nucleation – Classical theory of nucleation – Gibbs Thomson equation for vapour – Modified Thomson's equation for melt –Gibbs – Thomson equation for solution-Energy of formation of a nucleus-Spherical nucleus – Cylindrical nucleus – Homogeneous and Hetergeneous nucleation- Kinetics of crystal growth (basis only).

UNIT - III: SOLUTION GROWTH TECHNIQUES

Low temperature solution growth: Solution – Solubility and supersolubility – Expression of supersaturation – Mier's T- C diagram – Constant temperature bath and crystallizer – Seed preparation and mounting – Slow cooling and solvent evaporation methods – Gel growth – Various types – Structure of gel – Importance of gel technique- Chemical reaction method – Single and double diffusion method – Chemical reduction method – Complex and decomplexion method – Solubility reduction method – Advantages of gel method – High temperature solution growth – Hydrothermal growth – Flux growth.

UNIT - IV: MELT AND VAPOUR GROWTH TECHNIQUES

Phase diagram and phase rules (basic concept) – Melt techniques – Bridgman technique- Basis process – Various crucible design – Thermal consideration – Vertical Bridgman technique – Experimental arrangement – Czochralski technique – Experimental arrangement –Verneuil method – Vapour growth – Basics of vapour growth – Chemical Vapour Transport (CVT) - Experimental arrangement.

UNIT - V: ANLYTICAL TECHNIQUES

Characteristics-Physical parameters-Basic principles and description of techniques - X-rays - UV- IR- Visible- Raman and FTIR spectroscopy, DTA-TGA-DSC thermal studies- NMR Techniques- Dielectric studies- Photoconductivity studies-Microhardness studies-SEM and TEM techniques-NLO studies-Kurtz –Perry powder technique.

BOOKS FOR STUDY AND REFERENCES:

1. C. Kittel, Introduction to Solid State Physics Wiley Eastern, New Delhi (1977).
2.M. M. Woolfson, An Introduction to X-ray Crystallography (Cambridge University Press, Cambridge (1991).
3. S. O. Pillai, Solid State Physics (New Age International, New Delhi (1995).

4.N. W. Ashcrof and N. D. Mermin, Solid State Physics (Holt, Rinehart and Winston, Philadelphia).
5.J. S. Blakemore, Solid State Physics, Cambridge University Press, Cambridge (1974).
6. A. J. Dekker, Solid State Physics (McMillan, Madras (1971).
7. J.C. Brice, Crystal Growth Processes, John Wiley and Sons, New York (1986).
8. P.Santhana Raghagavan and P.Ramasamy, Crystal Growth Process and methods, KRU Publications, Chennai (2004).
9**.**Buckley. H.E., 'Crystal Growth', John Wiley and Sons, New York(1951).
10**.**Elwell.D and Scheel H.J., 'Crystal Growth for High Temperature Solutions', Academic Press Inc., London (1975).
11.Silverstein, R.M., Glayton Bassiler. G. and Mozill. T.C., Spectroscopic Identification of organic compounds, Fourth edition, John Wiley and sons, New York (1981).
12.Kurtz S.K. and Perry T.T., 'A powder technique for the evaluation of Nonlinear Optical Materials', J. Appl. Phys., Vol. 39,pp. 3798–38l3. (1968).
13.Anderson J.C., Dielectrics, Chapman and Hall, London, (1964).
14. Joshi V.N., 'Photoconductivity', Marcel Dekker, New York (1990).
15.Onitsch E.M., 'The present status of testing the hardness of materials', Mikroskopie, Vol. 95, pp. 12-14. (1956).

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ELECTIVE COURSE– IV: VIBRATIONAL SPECTROSCOPY

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Understand the basic concept to atomic spectra
CO2: Learn molecular vibrations
CO3: Study IR spectroscopy and its instrumentation techniques
CO4: Understand Raman spectroscopy and its theory
CO5: Study about basic principle of NMR and its instrumentation techniques

UNIT- I: CONCEPTS OF SPECTROSCOPY

Concepts of spectroscopy – Properties of electromagnetic radiation - Spectrum-different types of molecular energies- Electronic spectra of diatomic and poly atomic molecules – Importance of vibrational spectroscopy-Descriptions of vibrations-Fermi Resonance- Group frequencies- Coupled vibrations.

UNIT-II: MOLECULAR VIBRATIONS

Classification of the normal vibrations – Determining the symmetry types of the normal modes-Selection rules for vibrational transitions force constants –F and G matrix method- Over toners and combination bands-Internal and symmetry coordinates-Band assignments-Refinement of force constants.

UNIT -III: INFRARED SPECTROSCOPY

Principle of infrared spectroscopy – Molecular vibrations-Vibrational frequency-Number of fundamental vibrations-selection rules-Factors influencing vibrational frequencies-Infrared instrumentation-Sampling techniques-Finger print region-Important features of infrared spectroscopy-Applications of infrared spectroscopy-Interpreting an infrared spectrum.

UNIT-IV: RAMAN SPECTROSCOPY

Classical theory of Raman scattering-Quantum theory of Raman effect – Theory of Raman spectra-General selection rule for Raman scattering – Raman spectra of diatomic molecules-Vibrational Raman spectra of polyatomic molecules – Rule of mutual exclusion principle-Infrared and Raman spectra are complimentary-Structure elucidation by Raman spectroscopy-Instrumentation and sampling techniques-Importance of Raman spectra-Application of Raman spectroscopy.

UNIT- V: NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Principles – Origin of NMR- Modes of nuclear pin – Instrumentation – Measurements of NMR spectra – Relaxation process- Chemical shift – Shielding and deshielding effects – Factors affecting chemical shift – Anisotropic effects – Peak area and proton counting – splitting of the signals – Spin-spin coupling – Proton exchange reactions – Coupling constants – Other couplings.

BOOKS FOR REFERENCES:

1. Vibrational Spectroscopy – Theory and Applications, D.N. Sathyanaraya, New age International Publishers, New Delhi (2004).
2. Spectroscopy – Atomic and Molecular, Gurdeep R.Chatwal, Sham K. Anand, Himalaya Publishing House, Delhi (2004).
3. Modern Molecular Spectroscopy – H.S.Randhawa, Mac.Millan India Ltd. (2003).
4. Chemical Applications of Group Theory, F Albert Cotton, Wiley Eastern Ltd., New Delhi (1988).
5. Molecular Structure and Spectroscopy, G. Aruldhas, PHI Learning Private Limited, New Delhi (2009).

6. Gupta, S.L. Kumar, Sharma, Elements of Spectroscopy, Pragati Prakasham Publication, Meerut (2009).
7. P.S. Sindhu, Elements of Molecular Spectroscopy, New Age International (2007).
8. A.K. Chandra, Introductory Quantum Chemistry, Mc Graw Hill, New Delhi (2003).
9. C.N. Banwell, Elaine M., Mc Cash, Fundamental of Molecular Spectroscopy, Mc Graw Hill, New Delhi (2010).

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ELECTIVE COURSE– IV: THEORETICAL CHARACTERISATION OF AMINO ACIDS

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Study about the basics of thermodynamics, types of biomolecules and its importance
CO2: Understand about classification of amino acids and peptides
CO3: Study about equation of state
CO4:Understand about the basics of instruments to measure various parameters
CO5: Study about various analytical techniques.

UNIT - I: INTRODUCTION

Laws of thermodynamics – first, second, third and zeroth laws. – Laws of mass action – Measurements of pH – Identification of functional groups – Amines – Types of bio molecules – Importance of biomolecules.

UNIT - II: AMINO ACIDS AND PEPTIES

Amino acids: Structures, classification, physical and chemical properties. Titration curves of amino acids. Peptides: amides, peptide bonds, biological importance of peptides.

UNIT - III: EQUATION OF STATE

Introduction to L-J potential parameters – Chemical potential – Types of equations of state – Percus- Yevick , MCSL , MC- Analysis of equation of state - Applied to liquids.

UNIT - IV: MEASUREMENT BASICS

Sound velocity measurement using ultrasonic interferometer – Basic principles of Scanning Electron Microscope, Tunneling Electron Microscope, Scanning Transmission Microscope – Particle size determination methods.

UNIT - V: ANALYTICAL INSTRUMENTS

Basic principles and applications of Nuclear Magnetic Resonance – Circular Dicroism – Electron Spin Resonance - Basic ideas about COSPY and NOSOY peak formations in NMR.

BOOKS FOR STUDY:

1. Fundamentals of Biochemistry – O.P Agrawal, S Chand publ.
2. Essential of Biochemistry – M.C Pant, Tata Mc Graw Hill public.
3. Biophysical chemistry – Principles and techniques – Upadyay and Nath, PHI

BOOKS FOR REFERENCE:

1. Basic one and two dimensional spectroscopy – Horst Friebolin – VCH pub. (1991).
2. Principles and techniques of practical biochemistry – Wilson and Walker.

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ELECTIVE COURSE– IV: X– RAY CRYSTALLOGRAPHY AND MOLECULAR ANALYSIS

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Understand the about the basics of crystallography and its instrumentation
CO2: Understand about molecular isomerism and conformations
CO3: Know the various energy minimization methods
CO4: Know the fundamentals of structure based drug design
CO5: Experiment various crystal structure investigation methods

UNIT - I: X-RAY CRYSTALLOGRAPHY

Review of basic concepts of crystals- Crystal diffraction-Bragg's law - Reciprocal lattice- Structure factor-Data collection – Data reduction - Wilson plot - Scale factor and temperature factor - Crystal structure determination- Space group determination - Systematic absences - Phase problem - Method of solution- Patterson and Heavy atom method - Isomorphous and anomalous scattering methods-Direct methods - Structure solution and refinement – Reliability factor- Simple crystal growing techniques for crystallographic analysis.

UNIT - II: MOLECULAR ISOMERISM AND CONFORMATIONS

Molecular geometry – Conformation-Configuration- Isomerism-Asymmetric carbon – Chirality – Fisher convention – L and D system - R-S system –Amino acids – Peptide bond – Rigid planar peptide – Cis and trans configuration –Conformation- Torsion angles – Phi and Psi – Allowed conformation of a pair of linked peptide units –Steric hindrance – Hard sphere approximation – Contact criteria – Ramachandran diagram – Conformational energy.

UNIT - III: ENERGY MINIMIZATION METHODS

Description of various interactions by potential functions – Energy map – Minimization of energy - Force fields-Types-Components and characteristics of force fields **–** ab initio methods-Semi empirical approaches - Basis sets and Quantum mechanical force fields- Use of MOPAC.

UNIT - IV: STRUCTURE BASED DRUG DESIGN AND MOLECULAR SCREENING

Introduction to drugs - Classification of drugs - Drug receptor interactions – Applications of molecular modelling in drug discovery. Introduction to Quantitative Structure Activity Relationships (QSAR) - Applications in drug discovery - Software tools for QSAR - An overview of common descriptors with emphasis to structure based descriptors-Lipinski's rule of five- Use of SWISSADME (online tool).

UNIT - V: CRYSTAL STRUCTURE INVESTIGATIONS AND MOLECULAR ANALYSIS

Geometry analysis and Hydrogen bonding patterns (Weak and Strong) - Crystal packing- Use of ORTEP and PLATON. - Building a molecule for optimization studies- AVOGADRO, file format conversions-BABELWIN-Molecular binding-Binding sites detection – Docking- Auto Dock.

BOOKS FOR STUDY AND REFERENCE:

Relevant Chapters in

1. Elementary Crystallography, D. Velmurugan, MJP Publishers, Chennai (2008).
2.Carmelo Giacovazzo et al., Fundamentals of Crystallography, Third Edition Oxford University Press (2011).
3.K. I. Ramachandran, G. Deepa and K. Namboori. Computational Chemistry and Molecular Modelling , Springer Verlag , Berlin (2008).
4. Comba and Hambly, Molecular mechanics, Wiley VCH publishers (1998).
5. Anand Solomon, K, Molecular Modelling and Drug design. MJP Publishers, Chennai (2008).
6.Crystal Growth Process and methods, P.Santhana Raghagavan and P.Ramasamy. KRU Publications, Chennai (2004).
7. Tutorials from the Home pages of relevant Software packages/Tools (Internet).

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ELECTIVE COURSE– IV: ULTRASONICS AND INSTRUMENTATION

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Study about the basics of Ultrasonics and experimental techniques
CO2: Understand about various Acoustical parameters and theories
CO3: Study about the Material characterisation
CO4: Understand about the basic use of Ultrasound in the field of medicine
CO5: Study about IR and NMR spectroscopy and its instrumentation

UNIT- I: INTRODUCTION TO ULTRASONICS AND EXPERIMENTAL TECHNIQUES:

Equation of a progressive wave-Wave parameters-Wavelength-Amplitude-Frequency-Time period-Phase- Velocity-Types of Molecular interactions-Ultrasonic study of molecular interactions-Preparation of liquid mixtures-Mole fraction-Weight and volume fraction.

Experiment to determine velocity, density and viscosity-Interferometer- Continuous method- Specific gravity bottle method- Oswald viscometer method.

UNIT-II: ACOUSTICAL PARAMETERS AND THEORIES OF ULTRASONIC VELOCITY

Acoustical parameters from velocity and other data: Adiabatic compressibility-Acoustic impedance-Intermolecular free length-Molar volume-Free volume-Internal pressure-Classical absorption- Gibb's energy-Apparent molar compressibility.

Free length theory-Collision factor theory- Nomoto's relation.

UNIT -III: MATERIAL CHARACTERISATION

Introduction-Classification-Experimental techniques: sample preparation- Velocity, density and attenuation measurements. Micro structural characterisation-Grain size measurements-Attenuation-Back Scattering-Rayleigh surface waves -Recrystallisation -Evaluation of mechanical properties-Tensile strength-Hardness-Fracture toughness.

UNIT -IV: ULTRASOUND IN MEDICINE

Ultrasound in tissues- Transducers for medical imaging-mechanically scanned probes-Arrays-Linear and curvilinear array probes-Instrumentation – Signal processing and display-Scans and its types- A scan- B- scan – Time position scan-Doppler scan-Duplex scan-Clinical application of B scan (qualitative idea only).

UNIT -V: IR AND NMR SPECTROSCOPY

Requirements for IR radiation absorption-Origin of IR spectra Infrared spectrometer-Source-Monochromator-Sample-Detector-Amplifier - Double Beam Spectrophotometer-Examination of IR spectrum-Applications.

NUCLEAR MAGNETIC RESONANCE SPECTROSCOPY

Principle of NMR spectroscopy-Origin of NMR -NMR instrumentation-Measurement of NMR spectra -Tips for interpreting NMR spectrum-Limitations of NMR studies-Applications of NMR spectroscopy.

BOOKS FOR STUDY:

1. Baldevraj, V.Rajendran and P.Palanichamy, Science and technology of Ultrasonics, Narosa publications (2007) (Unit I to IV).
2. H. Kaur, Spectroscopy, Pragati Prakashan publications (2004) (Unit V only).

BOOKS FOR REFERENCE:

1. Fundamentals of Ultrasonics –Blitz.J, 2nd edition Butterworth London (1967).
2. Molecular Theory of Solutions, Prigogine I, North-Holland pub co, Amsterdam (1959).
3. Atomic and Molecular Spectroscopy, Gurdeep R.Chatwal, Sham K. Chand, Himalaya publishing house.

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ELECTIVE COURSE – IV: PARTICLE AND MATERIAL SCIENCE

Course Outcome:

After successfully completing the course, the scholar will be able to

CO1: Study about the basics of nucleon structure formation
CO2: Understand about various growth techniques
CO3: Understand about the basics of thin film techniques
CO4: Study about nano structures and its experimental methods
CO5: Study about various characterization techniques

UNIT -I: NUCLEON STRUCTURE FUNCTION

Quarks as the building blocks of hadrons - Baryon magnetic moments -Discovery of heavier quarks - Colour degree of freedom - Nucleon structure function - The Bjorken scaling - The Quark Parton model. DIS Experiments of polarized leptons on polarized nucleons - The statistical model of the nucleon.

UNIT- II: GROWTH TECHNIQUES

Low temperature solution growth: Solution - Solubility and super solubility – Expression of super saturation – Mier's T-C diagram - Seed preparation and mounting - Slow cooling and solvent evaporation methods - Principle – Various types – Structure of gel – Importance of gel – Experimental-procedure - Bridgman technique - Czochralski technique – Experimental arrangement – Growth process - Physical vapour deposition – Chemical Vapour Deposition (CVD) .

UNIT- III: THIN FILM DEPOSITION TECHNIQUES

Thin Films – Introduction to vacuum technology - Deposition Techniques - Physical Methods –Resistive heating, Electron beam gun, Laser gun evaporation and flash evaporations, sputtering - reactive sputtering, Radio-Frequency sputtering - Chemical methods – Spray pyrolysis – Preparation of transparent conducting oxides.

UNIT-IV: ZERO DIMENSIONAL AND ONE DIMENSIONAL NANO STRUCTURES

Synthesis of metallic nano particles, semiconductor nano particles and oxide nano particles (homogeneous nucleation). nano particles by heterogeneous nucleus: Aero sol synthesis – Spray pyrolysis- Nanorods: Evaporation, condensation growth, Vapor-Liquid-Solid growth, electro spinning – Lithography - Top down and bottom up approaches- Fullerenes- Properties of fullerenes-Carbon Nano Tubes (CNTs)- Types, properties, synthesis and applications of CNTs.

UNIT -V: CHARACTERIZATION TECHNIQUES

X – Ray diffraction (XRD) – Powder and single crystal - fourier transform infrared analysis (FT-IR) – Elemental analysis – Elemental dispersive X-ray Analysis (EDAX) - Scanning electron microscopy (SEM) – UV-Vis-NIR spectrometer – Etching (Chemical) – Vicker's micro hardness.

BOOKS FOR STUDY:

1. Modern Physics- R. Murugeshan and Kiruthiga Sivaprasath, S.Chand and Company, New Delhi (2010).
2. Nuclear Physics - V. Devanathan, Narosa Publishing House, New Delhi (2008).
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