

**JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY KAKINADA**  
**Syllabus for Pre-Ph. D Examination**  
**Physics**

<b>PAPER – II</b>		<b>Subject Code</b>
<b>S. No</b>	<b>Subject</b>	
1	NANO MATERIALS THEORY AND PHYSICS OF NANO-MATERIALS	<b>1310101</b>
2	ADVANCES IN FERRO ELECTRIC MATERIALS	<b>1310102</b>
3	THEORY OF COMPUTATIONS IN MOLECULAR SPECTROSCOPY	<b>1310103</b>
4	ACOUSTICAL SPECTROSCOPY INVESTIGATIONS IN LIQUIDS – I	<b>1310104</b>
5	LIQUID CRYSTALS-I	<b>1310105</b>

<b>PAPER – III</b>		<b>Subject Code</b>
<b>S. No</b>	<b>Subject</b>	
1	ADVANCES IN FERROELECTRIC MATERIALS – II	<b>1310201</b>
2	ACOUSTIC SPECTROSCOPY INVESTIGATIONS IN LIQUIDS-II	<b>1310202</b>
3	NANO – MATERIALS	<b>1310203</b>
4	THEORY OF COMPUTELION IN MOLECULAR SPECTROSCOPY	<b>1310204</b>
5	LIQUID CRYSTALS-II	<b>1310205</b>

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**Syllabus for Pre-Ph. D Examination**  
**Physics**

**PAPER – II**

**Nano materials**  
**Theory and Physics of Nano-materials**

**Unit 1**

**Concepts of Nano-technology**

Nano size, top-down and bottom-up approaches, size matters reduction of dimensionality and surface to volume ratio, changes to the system total energy, changes to the system structure, structural properties, thermal properties, chemical properties, mechanical properties, magnetic properties, optical properties and electronic properties of nano-scale systems

**Unit 2**

**Nano materials**

Introduction, materials used in nanotechnology, Fullerenes – discovery, variations of Bucky balls, Bucky tubes, Properties of Fullerenes - aromaticity, chemistry of Fullerenes, solubility of fullerenes and quantum mechanics of fullerenes, synthesis of nano-materials – ball milling and sol gel methods

**Unit 3**

**Carbon nanotubes**

Discovery, structure of nano tubes, Types of nano tubes-single walled nano tubes (SWNT) and multi walled nanotubes (MWNT), types of SWNT- chiral, armchair and zig zag, properties of nanotubes – strength, electrical conductivity, thermal conductivity, transport, optical activity and chemical activity.

**Unit 4**

**Theory of Nano tubes**

The continuum shell theories of mechanics of carbon nano tubes, parameterization of continuum theories for single wall carbon nano tube repeat space theory applied to carbon nano tubes, modelling and analysis of carbon nano tube buckling using thick shell theory – Effective medium theory of optical properties of CNTs. Theory of electric charge enhancements in carbon nano tubes.

**Unit 5**

**Synthesis of Nano tubes**

Growth mechanisms of CNT – tip growth and root growth, Arc Discharge method – synthesis of SWNT and MWNT, Laser Ablation method, Plasma Enhanced CVD, Laser Assisted Thermal CVD, and Flame synthesis, purification of CNTs – Oxidation, Annealing, Magnetic purification

**References**

1. Nano technology by William Illsey Alkinson, Jaico Books
2. Applicability of the continuum shell theories, VM Harik, TS Gate & MP Nemeth, NASA
3. Wondrous world of Carbon Nanotubes by M.Daenen and R.D. de Fouw

**Advances in Ferro Electric Materials**

**1. Dielectrics**

Review of Fundamentals – the three vectors D, E, and P. Dielectric susceptibility, Complex Dielectric constant, Macroscopic and Microscopic Electric fields, Clausius – Mossotti Relation, Polarization Mechanisms, Electronic, Ionic and Dipolar Polarizations and their temperature dependence Frequency Dependence of Dipolar Polarizability, Ionic Polarizability, Electronic Polarizability, Ferro electricity, Curie – Weiss law and Curie Temperature, Theories of Ferro electricity, Ferro electric Hysteresis, Classification of Ferro electric crystals, Ferro elasticity, piezoelectricity, Mathematical Description and Piezoelectric coefficients, pyroelectricity, pyroelectric responsivity, Pyroelectric Energy Conservation [1&2]

**2. Magnetic materials**

Quantum theory of Diamagnetism, Origin of paramagnetic moments – the Orbital Magnetic moment, the spin magnetic moment, the total magnetic moment, classical and quantum theory of para-magnetism, ferro-magnetism, Weiss theory of spontaneous magnetization, temperature dependence of spontaneous magnetization, Nature and origin of the Weiss Molecular Field theory, Exchange interaction, Hysteresis, Weiss theory of Hysteresis, Ferro magnetic Domains, Anti Ferro magnetism, Neel Temperature, Ferri magnetism, Molecular field theory of Ferri-magnetism, Ferrites – Spinel Inverse spinel and mixed ferrites [1&2]

**3. Diffusion in solids and sintering**

Diffusion in Crystalline solids, Laws Diffusion, Chemical Potential, Diffusional Flux Equations, Temperature Dependence of Diffusion coefficient, Determination of Activation Energy, Sintering-Driving Force for sintering, Mechanisms of sintering, Theoretical analysis of sintering, Numerical simulation of sintering, sintering Diagrams, Liquid Phase sintering – Elementary Features of Liquid phase sintering, stages of liquid phase sintering, The Basic mechanisms of liquid phase sintering, Hot pressing with a Liquid Phase, Activated Sintering [3 &4]

**4. Grain Growth and Microstructure Control**

Introduction, General Features of Grain Growth – Grain Growth and Coarsening, Driving Force and Grain Growth, Normal and Abnormal Grain Growth, Effect of Grain size on Properties, Attainment of High Density, Ostwald Ripening – The LSW theory, Ostwald Ripening Controlled by Interface Reaction, Time Dependent Ostwald Ripening, Normal Grain Growth in Dense solids, Computer Simulation of Normal Grain Growth, Abnormal Grain Growth in Dense solids – Causes of Abnormal Grain Growth, Grain Growth and Pore Evaluation in Porous Solids – Thermo dynamics of Pore Boundary interactions, Grain Growth in very Porous solids, Grain Growth in less Porous solids, Pore mobility, Structure Determination – Bragg's Law, Electron Diffraction, Neutron Diffraction, Mossbauer Effect [1 &3]

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**5. Conventional and Modern Physics of Ferroelectrics**

Theory of Polarization – A modern approach: Fallacy of Clausius – Mossotti Picture, Fallacy of Defining Polarization via the Charge Distribution, Landau Primer for Ferroelectrics – Introduction, Landau – Devonshire Theory: General Phenomenology, Second Order (Continuous) Transition, First order (Discontinuous) transition, Coupling to Strain, Soft Modes, Domains, Landau-Ginzburg Theory: General Considerations, Displacive and Order – Disorder Transitions, Diffuse Phase Transitions – Dielectric Relaxators, Recent Developments in Bulk Ferroelectricity, What causes Ferroelectricity and what causes Ferro magnetism? Multiferroics – The scarcity of Ferro magnetic Ferroelectrics, Magnetolectric coupling, composites [5 & 6]

**References:**

1. Introduction to Solid state Physics by Charles Kittel, Wiley Eastern Ltd, New Delhi
2. Solid state physics by R.L. Synghal Kedar Nath Ram Nath & Co, Meerut
3. Ceramic Processing and Sintering by M.N. Rahaman, Second Edition, Marcel Dekkar Inc, New York
4. Material science by Vijaya and Rangarajan, Tata McGraw Hill Publishing Company Ltd., New Delhi
5. Principles and Applications of Ferroelectrics and Related Materials by M.E. Lines and A.M. Glass, Clarendon Press 1977, Oxford
6. Physics of Ferroelectrics Modern Perspective by Rabe, Ahn, Jean Marc Triscon, Springer Series, 2007

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**Physics**

**THEORY OF COMPUTATIONS IN MOLECULAR SPECTROSCOPY [THEORY]**

**Unit 1**

**Infrared Spectroscopy**

Electromagnetic Spectrum – basic principles of vibrational spectroscopy, Infrared Spectroscopy – introduction, correlations of Infrared spectra with molecular structure, instrumentation, sample handling, quantitative analysis and applications

References: reference 6

**Unit 2**

**Vibrational Spectroscopy**

Diatomic molecules: Infrared spectra, Raman spectra, Anharmonicity, Vibration – Rotation spectroscopy

Reference: Chapter 6 of reference 1.

**Unit 3**

**Vibrational Spectroscopy**

Polyatomic molecules: Group vibrations, Normal vibrations of non – degenerate systems, Vibrational selection rules for infrared and Raman spectra, Vibration - rotation spectroscopy of linear molecules, Symmetric rotors, Spherical rotors and asymmetric rotors.

Reference: Chapter 6 of Reference 1

**Unit 4**

**X- ray diffraction, Scanning Electron microscopy**

X-ray diffraction from crystal planes, Reciprocal lattice, Interpretation of diffraction patterns, Determination of crystal structures, Crystal Symmetry, Point groups and Space groups, Electron matter interaction, Scanning electron spectroscopy.

Reference: Chapter 13, 21 and 22 of reference 2.

**Unit 5**

**Density functional theory**

Introduction to molecular electronic structure, abinitio methods, Semi empirical methods, Density functional theory methods, Molecular geometry, thermodynamic properties, Molecular vibrational frequencies, Computational programs, Performing abinitio calculations with Gaussian.

Reference: Chapter 15 and 16 of reference 5.

References:

1. Modern spectroscopy by J.M Holas (John Wiley & sons 2004)
2. Instrumental methods of analysis by WILLARD, MERRITE, DEAN AND SETTLE(CBS Publishers)
3. Vibrational spectroscopy theory and applications by D. N Satyanarayana (New Age International publishers).
4. Molecular Quantum mechanics by P. W. Atkins and R. S Friedman (Oxford University press)
5. Quantum Chemistry by IRA N. LEVINE VI edition 2009 (printice Hall India)
6. Fundamentals of molecular spectroscopy – Colin N Banwell and Elaine M Mccash, Tata McGraw Hill, New Delhi.

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**Syllabus for Pre-Ph. D Examination**  
**Physics**

**ACOUSTICAL SPECTROSCOPY INVESTIGATIONS IN LIQUIDS – I**

**Unit 1**

Characteristics of Ultrasonic waves, Equation of motion for plane waves, Specific acoustic impedance and intensity, Attenuation, Reflection and Refraction of plane waves. Ultrasonic transducers – piezoelectric, Magnetostrictive & electromagnetic.

**Unit 2**

Propagation of ultrasonic waves in liquids – velocities in liquids and liquid mixtures, absorption and dispersion in liquids, Thermal and structural relaxation in liquids. Measurements in liquids – Progressive wave method, Acoustic interferometer, Pulse technique & Optical methods.

**Unit 3**

Effect of temperature and pressure on the absorption coefficient, Theory of sound velocity: Rao's rule. Adiabatic compressibility, Intermolecular free length, Internal Pressure and their excess parameters.

**Unit 4**

The theories of static permittivity – Debye's theory of static permittivity & Onsager's theory of the internal field and permittivity. The statistical theories of non – polarisable dipoles – Kirk woods theory & Frohlich's theory.

**Unit 5**

Representation of permittivity in the complex plane, Debye's equations, Cole – Cole arc, Cole – Davidson arc & Distribution of relaxation times. Eyring's rate process theory of dielectric relaxation

**Unit 6**

1. Acoustic and thermodynamic investigations on binary mixture systems.

URL: <http://www.sciencedirect.com/science/article/pii/S0040603110001668>

2. Volumetric studies on binary liquid mixtures.

URL: <http://pubs.acs.org/doi/abs/10.1021/je900874z>

3. Molecular association studies in liquids.

URL: <http://pubs.acs.org/doi/abs/10.1021/je060379q>

4. Investigations on molecular interactions using relative permittivity measurements.

URL: <http://www.sciencedirect.com/science/article/pii/S0021961411002655>

5. Physico – Chemical, Solvent properties and applications of ionic liquids.

URL: [http://nopr.niscair.res.in/bitstream/123456789/2077/1/IJCA%2047A \(4\) %20495-503.pdf](http://nopr.niscair.res.in/bitstream/123456789/2077/1/IJCA%2047A%20(4)%20495-503.pdf)

**Books for Reference**

1. Ultrasonic methods and applications – J. Blitz Butterworth Public. & co 1971 (Units 1,2 & 3)
2. Physical Ultrasonics – R. T. Beyer & S. V. Letcher, Academic Press – London. 1969 (Unit 2)
3. Dielectric properties and molecular behaviour – N. E. Hill, W. E. Vaughan, A. H. Price & M. Davies – Van Nostrand Reinhold Company, 1969. (Unit 4 & 5)
4. Dielectric Behaviour and Molecular structure – C. P. Smyth – McGraw Hill. (Units 4 & 5)

**Liquid Crystals-I (Theory)**

**UNIT I**

Chemical constitution - Thermotropic Liquid Crystals - Nematics, Smectics, Cholesterics and Disc like molecules - Achiral and Chiral molecules - Occurrence of Ferroelectricity - Supra-molecular Design of molecules - Banana Molecules, Lyotropic Liquid Crystals - Monolayer and Bilayer arrangements - Monotropic and Enantiotropic Liquid Crystals - Bridging Groups - Chemical Moieties and their influence for mesomorphism.

**UNIT II**

Microscopic investigations including basic concepts - Phenomenology and Morphology - Polymorphism - Boundary effects - Textures - Homogeneous and Homeotropic textures of Nematic and Smectic phases.

**UNIT III**

Theories of Liquid Crystalline state - Swarm theory - Continuum theory -Maier Saupe theory (Mean field) - Landu de Gennes theory - Pre-transitional Effects - McMillan theory of smectic-A phase and its developments.

**UNIT IV**

Electric and Magnetic field effects - Elastic Deformation (Frederick's deformation) - Magnetic field effects (temperature) on Nematic and Smectics -Electric field effects - Domains - DSM - Loops - Electro Hydrodynamics instabilities.

**UNIT V**

Hydrogen bonding and supramolecular liquid crystals: Chemical moieties - shape based classification of LCs - Metallo - Mesogens - Bent liquid crystals - Hydrogen bonding liquid crystals - chemical moieties and interaction effect on physical properties - types of HB LCs - Polycatenar liquid crystals

**Text Books & References:**

1. *'The Physics of Liquid Crystals'* by P.G.de Gennes, Ed: Marshall and Wilkinson, Clarendon Press, Oxford, U.K.
2. *'Introduction to Liquid Crystals'* by E.B.Priestley, Plenum Press.
3. *'Liquid Crystals'* by S.Chandrasekh Cambridge Univ. Press.
4. *'The Molecular Physics of Liquid Crystals'* by G.R.Luckhurst and G.W.Gray, Academic Press, New York, U.S.A
5. *'Hand Book of Liquid Crystals'* by T.Kato, Ed: D.Demus, J.Goodby, G.W.Gray, Ed: H.W.Spiess and v.vn (Weinheim: Wiley-VCH). 1998.
6. *'Thermotropic Liquid Crystals - Recent Advances'* Ed: ARamamoorthy. Springer Press.
7. *'Alignment Technology and Applications of Liquid Crystal Devices'* by Kohki Takatoh, Masaki Hasegawa et ai, Taylor & Francis press.
8. *'Ferroelectric Liquid Crystals - Principles, Propeties and Applications'* by J.W.Goodby, R.Blink, N.AClark, S.T.Lagerwall et al.
9. *'Ferroelectric Liquid Crystals'* by B.Zeks and R.Blink, Gordon & Breach.
10. H.Kihara, T.Kato, T.Uryu, S.Ujiiie, U.Kumar, J.M.J.Frechet, D.W.Bruce and D.J.Price, *Liq. Cryst.*, **21**, (1996) 25; Z.Siderotou, D.Tsiourvas, C.M.Paleos and ASkoulios, *Liq. Cryst.*, **22**, (1997) 51; C.M.Paleos and D.Tsiourvas, *Liq. Cryst.*, **28**, (2001) 1127.
11. T.C.Lubensky and L.Radzihovsky, *Phy. Rev. E.*, **66**, (2002) 031704.

## PAPER – III

### Advances in Ferroelectric Materials - II (FABRICATION, CHARACTERIZATION AND APPLICATIONS)

#### Unit 1

##### Ferroelectric Materials

General Classification of Ferroelectric Materials: Corner Sharing Octahedra, Tetrahedral Oxygen Groups, Hydrogen Bonded Compounds and polymers, properties and Characteristics of some Important Ferroelectric Materials: The Ferroelectric perovskites – Barium Titanate, Lead Titanate, Sodium Niobate, Lithium Niobate, Antiferroelectric and cell Doubling perovskites – Lead Zirconate, Lead Zirconate Titanate, Tungsten Bronze Type Structures – Strontium Barium Niobate, Barium Sodium Niobate, other Ferroelectrics-Magnetic Ferroelectrics, Electronic Ferroelectrics and Non Bulk Ferroelectrics, Multiferroics –  $\text{BiFeO}_3$  and  $\text{YMnO}_3$  (3&4)

#### Unit 2

##### Fabrication of Ceramic Materials

Powder Preparation by Mechanical Methods: Solids State Reaction (Stoichiometry, Calcination, Sintering etc.) – Ball Milling, Hardness, Considerations, Types of Hardness, Density and Hardness, Normalized Density, Knoop Hardness and Normalized Density, Powder preparation by Chemical Methods – Sol Gel Processing : Preparation Techniques, Thin Film Growth of Complex Oxides: Vacuum Chamber, Temperature Control and Monitoring, Pulsed Laser Deposition – Laser, Targets, Ablation Process and Film Growth using PLD, Sputter Deposition – Sputtering Process, The Sputtering of Insulators, Process Gas, Oxide Molecular Beam Epitaxy – Hardware, RHEED, Fundamentals of Growth (1,2 &3)

#### Unit 3

##### Structure and Microstructure Characterization

X-Ray Diffraction : Experimental Methods – Laue Method (Introduction, Cameras, Specimen Holders, Collimators and Shapes of Laue Spots), Debye Scherre Method (Specimen Preparation and Film Loading) Grain Size, Particle Size, Preliminary Treatment of Data, Indexing Patterns of Cubic Crystals, Indexing Patterns of Non Cubic Crystals – Graphical Methods, Indexing Patterns of Non Cubic Crystals – Analytical Methods, Determination of Number of Atoms in a Unit Cell, Determination of Atom Positions, Microstructure Determination Techniques – Scanning Electron Microscopy, Scanning Tunneling Microscopy and Transmission Electron Microscopy (5)

#### Unit 4

##### Other characterization Techniques

Small Signal Dielectric Measurements, Pyroelectric Measurements – Voltage Responsivity, Current Responsivity and Normalized Detectivity, Experimental Constraints, Measurement of Piezoelectric Coefficients – Experimental Techniques (Berlin Court D-33 Meter etc.), Hysteresis Measurement, Experimental Techniques for DC Resistivity Measurement- Two Probe Method and Four Probe Method, Determination of Chemical Composition – Optical

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## Syllabus for Pre-Ph. D Examination

### Physics

Atomic Spectroscopy and X-Ray Fluorescence Spectroscopy, Thermal Analysis –  
Differential Thermal Analysis and Differential Scanning Calorimetry (2&4)

#### Unit 5

##### Application of Ferroelectrics

Sensors, Ultrasonic Cleaners, Flow Detectors, High Voltage Generators, Electromechanical Transducers, Actuators, Optical Information Storage Devices, Underwater Acoustics, Heterodyne Detection, Pyroelectric Imaging, Ferroelectric Memory Technology – Electrically Read Memories, Optically Read Memories, High Capacity Memories, Electro – Optic Modulators, Travelling Wave Modulators, Potential Future Applications (Ferroelectric Nano Structures, Field Effect Devices, Ferroelectric Device Fabrication using Atomic Force Microscopy, Ferroelectric Cooling Devices) (4)

##### References

1. Some Fundamentals of Mineralogy and Geochemistry by L. Bruce Railsback
2. Ceramic Processing and Sintering by M.N. Rahaman, Second Edition, Marcel Dekker Inc. New York.
3. Physics of Ferroelectrics - Modern Perspective by Rabe, Ahn, Jean Marc Triscon, Springer Series, 2007
4. Principles and Applications of Ferroelectrics and Related Materials by M.E. Lines and A.M. Glass, Clarendon Press 1977, Oxford.
5. X-Ray Diffraction by B. D. Cullity, Adison Wesley Publishing Company, Inc. 1956, Masachusetts.

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**Physics**

**ACOUSTIC SPECTROSCOPY INVESTIGATIONS IN LIQUIDS-II**  
**(COMPUTATIONAL STUDIES)**

**Unit 1**

**Studies on Hydrogen bonding**

Introduction, properties of Hydrogen bonded substances, importance of the Hydrogen Bond. Intramolecular Hydrogen bonds – some examples, comparison of properties. Electrostatic theory of Hydrogen bond formation, heat of formation.

**Unit 2**

**Infrared Spectroscopy**

Electromagnetic Spectrum – basic principles of vibrational spectroscopy. Infrared spectroscopy – introduction, correlations of Infrared spectra with molecular structure, instrumentation, sample handling, quantitative analysis and applications.

**Unit 3**

**Raman Spectroscopy**

Introduction, difference between Raman and infrared spectra, quantum mechanical description of the Raman effect, selection rules, depolarisation ratio, resonance Raman effect. FT Raman – instrumentation, sample handling techniques and applications.

**NMR**

Principle of Nuclear Magnetic Resonance, NMR experimental technique, chemical shift, application to H-bonding studies.

**Unit 4**

**Computational techniques (part – 1)**

Hartree -Fock Theory – introduction, Hartree-Fock Equation, restricted and unrestricted Hartree- Fock models, steps for the HF calculation, Koopman's theorem. Semi empirical methods – introduction, Modified Neglect of the Diatomic Overlap method, Austin Model 1 Method, Parametric Method 3 Model, Comparisons of Semi empirical methods.

**Unit 5**

**Computational techniques (part -2)**

Ab Initio Method – introduction, Many – Body Perturbation Theory, Moller - Plesset Perturbation.

Density Functional Theory – Electron density, pair density, development of DFT, density functionals, The Becke Exchange Energy Functional and the Potential, The Lee, Yang, and Parr correlation energy functional and the potential, applications of DFT.

Introduction to the modeling software packages – Gaussian 09, Spartan 08 and MOPAC.

**Unit 6**

1. Hydrogen bonded studies in liquid mixtures.

URL: <http://WWW.publish.csiro.au/paper/CH9661129.htm>

2. Experimental Spectroscopic Studies

URL: <http://WWW.sciencedirect.com/science/article/pii/S0022286011006107>

3. NMR Spectra analysis

URL: <http://WWW.sciencedirect.com/science/article/pii/S0022286010005934>

4. F T I R and FT- Raman Spectra – Computational studies.

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**Physics**

URL:

<http://nopr.niscair.res.in/bitstream/123456789/10622/1/IJPAP%2048%2812%29%20869-874.pdf>

5. Computational spectroscopic studies.

URL: <http://onlinelibrary.wiley.com/doi/10.1002/jrs.2520/abstract>

**Books for Reference**

1. The Hydrogen Bond – G. C Pimentel & A. L. McClellan W. H. Freeman & Company, Sanfrancisco & London. (Unit 1)
2. An Introduction to Hydrogen Bonding- A. J. George, Oxford University press, Oxford, England, 1997. (Unit 1)
3. Organic Spectroscopy Principles and Applications – Jag Mohan, Narosa Publishing House, New Delhi. (Unit 2 & 3)
4. Fundamentals of molecular spectroscopy – Colin N Banwell and Elaine M Mccash, Tata McGraw Hill, New Delhi. (Units 2 & 3)
5. Molecular Structure and Spectroscopy – G. Aruldhas, Prentice Hall India, New Delhi. (Unit 2 & 3)
6. Computational Chemistry and Molecular Modeling – K. I. Ramachandran, G. Deepa, K. Namboori, Springer – Verlag Berlin Heidelberg. (Unit 4 &5 )
7. Molecular Modeling: Principles and Applications – Andrew R. Leach, 2<sup>nd</sup> Ed, Prentice Hall, 2001. (Unit 4)

**JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY KAKINADA**

**Syllabus for Pre-Ph. D Examination**

**Physics**

**Nano – Materials**

**(INSTRUMENTS AND APPLICATIONS)**

**Unit 1:**

Nanoelectronics: Fabrication of Integrated Circuits, substances deposited for integrated circuits – polysilicon, silicon dioxide, metals, Microelectromechanical Systems(MEMS) – materials in MEMS technology, MEMS processes – deposition, photolithography, wet and dry etching, Applications of MEMS.

**Unit II:**

Nanoelectromechanical Systems (NEMS): Nanowires- Production of nanowires, conductivity of nanowires, Nanocircuits – Production of nanocircuits, applications of nanocircuits, Quantum Wires – CNTs as quantum wires, Quantum Wells –fabrication of quantum wells, Applications of quantum wells

**Unit III:**

Molecular Nanotechnology: Smart materials and nanosensors, nanofactories, self replacing machines, types of molecular machines – synthetic, biological and theoretical machines, Nanorobotics – theory, Nubots, applications, DNA nanotubes, DNA Polyhedra, DNA nanomechanical devices, potential social impacts of molecular nanotechnology.

**Unit IV:**

Analytical instruments: Atomic Force Microscope(AFM) – Principle, imaging modes, tapping modes and applications, Scanning tunneling microscope(STM) – tunneling, working; STM related techniques; Electron beam lithography, ion beam sculpting.

**Unit V:**

Nano medicine: Drug delivery, nano particles as controlled drug delivery devices, Surgery, Nano particle targeting, nano Robots, cell repair machines, Insulin loaded Nano capsules, Nano bio technology and applications.

**Reference Books:**

1. Nanotechnology by William Illsey Atkinson, Jaico Books.
2. Principles of Nanotechnology by Phani Kumar
3. Nanotechnology by Ratner and Ratner
4. Wondrous world of Carbon Nanotubes by M. Daenen and R.D. de Fouw

**JAWAHARLAL NEHRU TECHNOLOGICAL UNIVERSITY KAKINADA**  
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**Physics**

Theory of Computation in Molecular Spectroscopy  
[EXPERIMENTAL METHODS AND INSTRUMENTATION]

Unit 1:

Experimental methods and instrumentation:

Electromagnetic spectrum, general components of absorption experiment, Fourier transformation and interferometers, Infrared, Visible and ultraviolet radiation, Comn microscopy ponents of absorption experiments in the regions of far infrared, near infrared and mid infrared, Visible and near ultraviolet.  
Reference: chapter 3 of reference1.

Unit 2:

Atomic absorption spectroscopy:

Spectrophotometers for near infrared mid infrared visible and ultraviolet regions.  
Reference: Chapter 3 of reference1.

Unit 3:

Electro analytical methods:

Conductivity: measurement of conductivity, conduction in amorphous and imperfectly crystalline materials.

A.C. Conductivity: Amorphous and imperfectly crystalline materials, Electro chemical cells, Current potential relationships, Classification of electrodes, Ion selective electrodes, voltammetric techniques.  
Reference: Chapter 13,21 and 22 of reference 2.

Unit 4:

Group theoretical applications of Vibrational spectroscopy:

Symmetry of translation, Rotational and molecular polarizability, Factor groups and site groups, Classification of normal vibrations, selection rules for vibrational transitions, Vibrational wave functions and Spectral activity, infrared absorption, raman scattering, Overtone and combination bands, Linear molecules.

Reference: Chapter 3 and 4 of reference3

Unit V:

Molecular Electronic structure methods:

Hartree Fock theory:

The Born- Oppenheimer approximation, Molecular Orbital theory of diatomic molecules, molecular Orbital theory of Polyatomic molecules, Hartree Fock's self consistent field method, Restricted and unrestricted Hatree Fock calculators, Selection of basis sets, Electron correlation, Configuration interaction.

Reference: Chapter 8 and 9 of reference 4.

References:

7. Modern spectroscopy by J.M Holas (John Wiley & sons 2004)
8. Instrumental methods of analysis by WILLARD, MERRITE, DEAN AND SETTLE(CBS Publishers)
9. Vibrational spectroscopy theory and applications by D. N Satyanarayana (New Age International publishers).
10. Molecular Quantum mechanics by P. W. Atkins and R. S Friedman (Oxford University press)
11. Quantum Chemistry by IRA N. LEVINE VI edition 2009 (printice Hall India)
12. Fundamentals of molecular spectroscopy – Colin N Banwell and Elaine M Mccash, Tata McGraw Hill, New Delhi.

**Liquid Crystals-II (Applications)**

**UNIT-I**

Thermodynamic properties - Theory of phase transitions - Pre-transitional phenomena - Calorimetric measurements - Molar heat - Transition entropy and Enthalpy.

**UNIT-II**

Optical properties - Birefringence - Rayleigh's Scattering - UV and visible absorption spectroscopy - IR spectroscopy.

**UNIT-III**

Liquid Crystal displays - Electro-optic phenomena - Field induced Birefringence - Twisted Nematics - Guest Host effect - Cholesteric to Nematic transition - Storage mode - Display life - Alignment of Liquid Crystal - Homogeneous and Homeotropic.

**UNIT-IV**

Technical applications - Thermography - Electro-optic display devices - Holography - Interferometry and other applications

**UNIT-V**

Electro-optic Modulators with liquid crystals - Ferroelectricity in smectic liquid crystals - surface Stabilized Switching mechanism in- Liquid Crystals - Polarization switching - Threshold less switching - V-shaped switching.

**Text Books & References:**

1. *'The Physics of Liquid Crystals'* by P.G.de Gennes, Ed: Marshall and Wilkinson, Clarendon Press, Oxford, U.K.
2. *'Introduction to Liquid Crystals'* by E.B.Priestley, Plenum Press.
3. *'Liquid Crystals'* by S.Chandrasekh Cambridge Univ. Press.
4. *'The Molecular Physics of Liquid Crystals'* by G.R.Luckhurst and G.W.Gray, Academic Press, New York, U.S.A
5. *'Hand Book of Liquid Crystals'* by T.Kato, Ed: D.Demus, J.Goodby, G.W.Gray, Ed: H.W.Spiess and v.vn (Weinheim: Wiley-VCH). 1998.
6. *'Thermotropic Liquid Crystals - Recent Advances'* Ed: ARamamoorthy. Springer Press.
7. *'Alignment Technology and Applications of Liquid Crystal Devices'* by Kohki Takatoh, Masaki Hasegawa et ai, Taylor & Francis press.
8. *'Ferroelectric Liquid Crystals - Principles, Propeties and Applications'* by J.W.Goodby, R.Blink, N.AClark, S.T.Lagerwall et al.
9. *'Ferroelectric Liquid Crystals'* by B.Zeks and R.Blink, Gordon & Breach.
10. H.Kihara, T.Kato, T.Uryu, S.Ujiie, U.Kumar, J.M.J.Frechet, D.W.Bruce and D.J.Price, *Liq. Cryst.*, **21**, (1996) 25; Z.Siderotou, D.Tsiourvas, C.M.Paleos and ASkoulios, *Liq. Cryst.*, **22**, (1997) 51; C.M.Paleos and D.Tsiourvas, *Liq. Cryst.*, **28**, (2001) 1127.
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