M.Tech. Nano Electronics and Nano Engineering 2022

This is a two-year course in *Nano Electronics and Nano Engineering* with a focus on applications in nanoelectronics, optoelectronics, materials sciences and energy sciences. Considerable research over the past decade has shown that nanomaterials can play a significant role in the above applications through use of nanoparticles, thin films and composites and materials with nano and mesoporous architectures. In the first year, this course provides a strong fundamental understanding of the processing and properties of such materials and the physics and chemistry behind use of such materials in device applications, and the physics of the devices themselves. Apart from those basic courses, core courses dealing with design of nanosystems, nanomaterials and their processing, properties and characterization, as well as on the applications of nanomaterials will be taught. Each student will have a thesis requirement involving one year of hands-on independent research experience in the advanced labs.

M. Tech in NanoElectronics and NanoEngineering

First Semester

Course Code	Type	Course Title	LTP	Credits
22NE601	FC	Statistical Data Analysis	101	2
22NE602	SC	Nanomaterials: Synthesis and Characterization	300	3
22NE603	SC	Nano- Opto- and Bio-electronic Devices	300	3
21HU601	HU	Amrita Values Programme	P/F	
21HU602	HU	Career Competency-I	P/F	
22AVP103		Mastery Over Mind	102	2
22NE681	SC	Lab-I: Optoelectronics Lab	004	2
22NE682	SC	Lab-II: Nanomaterials	004	2
		Electives Select (2 courses out of 3) 22NE631 – Solid State Phenomena at Nanoscale 22NE632 – Quantum Science 22NE633 – Modern Concepts in Materials Science	3 0 0	6
			Total Credits	**20**

Second Semester

Course Code	Type	Course	LTP	Credits
22NE611	SC	NanoEngineering Applications	201	3
22NE612	SC	VLSI Technology and Design	300	3
21HU603	HU	Career Competency-II	0 0 2	1
22NE683	SC	Lab-III: Nanoelectronics and Nanofabrication	004	2
22NE684	SC	Lab IV: NanoEnergy Devices	004	2
22NE613	FC	Ethics in Research and Research Methodology	101	2
		Electives Select (2 courses out of 4) 22NE641 – Emerging Nano-manufacturing Technologies 22NE642 – Polymeric Nanomaterials 22NE643 – Nanophotonics 22NE644 – Digital Electronics	3 0 0	6
			Total Credits	**19**

Third Semester

Course Code	Type	Course	LTP	Credits
22NE798	P	Dissertation	0 0 20	10
		Electives Select (2 courses out of 3) 22NE731 – Nanocarbon and Nanocomposites 22NE732 – Nanosensors 22NE733 – Computational Methods for Condensed Matter	3 0 0	6
			Total Credits	**16**

Fourth Semester

Course Code	Type	Course	LTP	Credits
22NNE699	P	Dissertation	0 0 32	16
Total Credits				**16**
Overall Credits				**71**

22NE601 Statistical Data Analysis 1-0-1 2

Pre-requisites: Undergraduate level basic maths, physics, chemistry and biology

Total number of classes: 30

Course Outcomes:

- *The basic concepts of statistics and the need for statistical methods in research*
- *Data Analysis Methods*
- *The fundamental theory of probability and standard distributions*
- *Tests of Significance used in Statistical analysis*
- *The different types of multivariate analysis used in research*
- *Practical analysis of data using standard softwares like SPSS, SAS*
- *Practical understanding of Descriptive Data Analysis, Sampling Theory, Biostatistical Inference, Testing of Hypotheses, Nonparametric Methods and Multivariate Regression Analysis*

Course Contents:

Unit-1 (6 Lectures)

Introduction to Statistics-Need for Statistical Methods –Their uses and Misuses, Types of Variables, Data collection Methods, Population and Sample.

Descriptive Data Analysis Methods- Statistical Tables, Diagrams & Graphs, Measures of Averages, Measures of Dispersion, Correlation Analysis Methods, Regression Analysis Methods.

Unit-2 (6 Lectures)

Theory of probability and Standard Distributions - Binomial, poisson& Negative Binomial, Standard univariate continuous distributions – Normal, Log normal & Exponential. Sampling distributions – Chi- square distribution and F & 't' distributions.

Unit-3 (6 Lectures)

Tests of Significance of Statistical Hypotheses- Concept of Statistical Hypotheses –Null and Alternative hypotheses, Type I and Type II errors, Significance level, Critical region and Power of a test , P- value and its interpretation; Large and Small Sample Test – Normal test, Student's 't' test, Chi-square tests, Analysis of variance.

Unit-4 (6 Lectures)

Nonparametric methods-Non-parametric methods for estimation, Methods for tests of significance for the independent and correlated samples, Nonparametric Methods for more than two populations.

Multivariate analysis Methods- Principles of Multivariate analysis, Multivariate regression analysis, Multivariate logistic regression analysis.

Unit-5 (6 Lectures)

Practicals- (Statistical Software to be used: SPSS & SAS): (i) Practicals in Descriptive Data Analysis Methods, (ii) Practicals in Sampling Theory, (iii) Practicals in Biostatistical Inference, (iv) Practicals in Testing of Hypotheses, (v) Practicals in Nonparametric Methods, (vi) Practicals in Multivariate Regression Analysis.

TEXT BOOKS/REFERENCES:

1. *Statistical Techniques for data Analysis: J.K. Taylor & Cheryl C, 2004 Chapman & Hall (CRC).*
2. *Performing Data Analysis Using IBM SPSS: Lawrence S Meyers, 2015, John Wiley.*

22NE602 Nanomaterial Synthesis & Characterization 3-0-0 3

Pre-requisites: Basic physics, chemistry and biology

Total number of classes: 45

Course Outcomes:

- *To understand various chemical synthesis (Bottom-up) of diverse types of nanomaterials (0D, 1D and 2D)*
- *To understand various physical methods (Top-down) of fabricating nanomaterials and nanostructures*
- *Decipher information on the various class of nanomaterials based on composition, shape and size (1D, 2D, 3/0D nanostructures)*
- *To understand the application potential of nanomaterials based on their unique properties and importance of selecting appropriate synthesis methods that will suit the specific application.*
- *To learn the fundamental principles of characterizing nanomaterials for their morphology, structure, chemistry and functionality through diverse methods of microscopy, spectroscopy, scattering and diffraction.*

Course content:

Nanomaterial Synthesis:

Unit 1 (5 lectures)

Synthesis of nanomaterials: Basic chemistry concepts, Inorganic, organic synthesis and analytical chemistry methods, concepts of precipitation reaction, mechanisms of nanocrystal growth, LaMer theory, Oswald ripening, coalescence

Unit 2 (5 lectures)

Bottom-up synthesis approaches – Nanoprecipitation reaction, synthesis of zero-dimensional metal, metal oxides, semiconductor nanoparticles by nanoprecipitation routes, high-pressure homogenization

Unit 3 (5 lectures)

Bottom-up synthesis approaches- Micro-emulsion route of synthesis, basic concepts of surfactant, emulsion, micelles, reverse micelles, critical micellar concentration, micro-emulsions: water-in-oil and oil-in-water emulsions, double emulsion and applications

Unit 4 (4 lectures)

Bottom-up synthesis approaches: Sol-gel method, hydrolysis and condensation, Self-assembly, Kinetically Confined Synthesis of Nanoparticles

Unit 5 (4 lectures)

Template-based synthesis; Synthesis of one dimensional nanosystems by different routes – VLS and SLS methods, Synthesis of two dimensional nanosystems

Unit 6 (5 lectures)

Top-down approaches: Fundamentals of nano–thin film Growth; Vapor phase deposition methods - Physical and chemical vapor phase methods; Langmuir-Blodgett Films; Electrochemical Deposition; laws of electrolysis and deposition

Characterization:

Unit 7: Structure, Morphology and Surface **(10 lectures)**

Crystal structure, Lattice parameters, nanoparticle size by Debye-Scherrer's formula. Working principles of the Scanning electron microscope and Transmission electron Microscope, particle size Dynamic Light scattering, Elemental analysis using energy dispersive X-ray analysis, Atomic absorption and inductively coupled Plasma. Fundamental working principles of scanning probe microscopy (STM) Atomic Force Microscopy, confocal fluorescence microscopy

Unit 8: Spectroscopy **(7 lectures)**

Fundamentals of spectroscopy, vibrational and rotational spectroscopy, Nanomaterials analysis using UV-VIS, Infrared & Raman spectroscopy, Surface enhanced Raman spectroscopy using nanotechnology. FTIR and NMR spectroscopy, Basic principles and applications of Mass spectrometry, chromatography and High-pressure Liquid chromatography in nanomaterial or nanomedicine characterization.

References

1. *Nanomaterials – An introduction to synthesis, properties and applications, D. Vollath, Wiley-VCH, Second Edition 2013.*
2. *G. Cao, Nanostructures and Nanomaterials – Synthesis, Properties and Applications, Imperial College Press 2006.*
3. *Elements of X-ray Diffraction, B. D. Cullity and S. R. Stock (Pearson)*
4. *Physical Principles of Electron Microscopy, R.F. Egerton (Springer)*
5. *Scanning Probe Microscopy and Spectroscopy, D. A. Bonnell (Wiley)*
6. *Fundamentals of Molecular Spectroscopy, C. N. Banwell (McGraw Hill)*
7. *Nanostructured materials: Processing, Properties and Potential Applications, Edited by Carl. C. Koch, Noyes Publications, 2002.*
8. *Materials Science and Engineering – An Introduction, William D Callister, 12th Edition, John Wiley (Available in Amazon India, Rs. 287)*

22NE603 Nano- Opto- and Bio-electronic Devices 3-0-0 (3 Credits)

Pre-requisites: Basic maths, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Familiarity with fundamental concepts related to material science of semiconductors.*
- *Get introduced crystal structures relation with fundamental aspects of atomic bonds and energy bands.*
- *Bulk semiconductors and their significance along with size effects and applications.*
- *Understand the influence of size effects on charge transport characteristics under various circumstances.*
- *Will be able to identify and choose suitable semiconductor nanostructures for different applications as required.*
- *Estimate the various physical parameters that are related to semiconductor nanostructures for example charge carrier mobility, conductivity and sheet resistance.*
- *Get introduced to emerging atomically thin nano-semiconductors such as 2D layered functional materials from current research literature.*
- *Understand the basics of spintronics and spintronic devices*
- *Get a brief idea of bioelectronics and its applications.*

Course content:

Unit-1: Introduction to semiconductors and properties (12 lectures)

Review of semiconductors, low dimensional semiconductors and materials, transport in nanostructures, Electron flow in solids, diffusive and ballistic electron transport, Coulomb blockade, hall-effect and quantum hall-effect, optical and electro-optic processes in heterostructures.

Unit-2: Semiconductor devices (12 lectures)

Nanoelectronic devices: heterojunction bipolar transistor, hot electron transistors, single electron transistors, resonant tunnelling transistors, low dimensional semiconductor lasers: quantum-well lasers, quantum dot lasers, vertical cavity surface emitting lasers, low dimensional photodetectors and modulators.

Unit-3: Advanced materials for nanoelectronics and optoelectronics (5 lectures)

2D materials (Graphene QDs, TMDs, MXenes… etc.) electronic, photonics and optoelectronics applications.

Unit-4: Spintronics and devices (8 lectures)

Spintronics: GMR, TMR, spin injection and detection, magnetic tunnel junctions, dilute magnetic semiconductors and spintronic devices.

Unit-5: Bioelectronics (5 lectures)

Bioelectronic devices: biosensors, micro-fluidics, biophysical concepts and methods, analytical electrochemistry, biomolecular electronics, BioNano machines.

Unit-6: Industry relevance analysis (3 lectures)

Industrial relevant failure analysis, metrology and device characterizations.

TEXTBOOKS/ REFERENCES:

1. *Nanotechnology for Microelectronics and Optoelectronics by Raúl José Martín-Palma, José Martínez-Duart, Fernando Agullo-Rueda, Elsevier (2006).*
2. *Introductory Bioelectronics: For Engineers and Physical Scientists by Ronald R. Pethig (Author), Stewart Smith, Wiley (2012).*
3. *Spintronics: Fundamentals and Applications by Igor Zutic, J. Fabian, and S. Das Sarma, Rev. Mod. Phys. 76, 323 (2004).*

21HU601 Amrita Values Program P/F

Pre-requisites: Basic understanding of Indian culture and values

Total number of classes: 15

Course Outcomes:

- *The basic concept of culture and values*
- *The relationship of culture with education, research, spirituality*
- *How culture is linked with gender, especially women*
- *The influence of media and politics in culture*

Course Content:

Unit-1 (3 Lectures)
Culture – definition and scope. Values and culture, cultural freedom
Culture and Education

Unit-2 (4 Lectures)
Culture of Research – creativity and responsibility in research
Spirituality and Culture – spirituality as a way of life, spirituality and religion

Unit-3 (4 Lectures)
Culture and women – gender oppression, motherhood
Culture and the Media

Unit-4 (4 Lectures)
Culture and Politics – national values and political harmony
Philosophy and Culture, epistemology

21HU602 Career Competency – I P/F

Pre-requisites: Basic understanding of the importance of career in life

Total number of classes: 15

Course Outcomes:

- *Effectively improve employability in the professional world.*
- *Gives training to assist the student to prepare for interviews*

Course Content:

Unit-1: Soft Skills (5 Lectures)

Introduction to 'campus to corporate transition':

Communication and listening skills: communication process, barriers to communication, verbal and non-verbal communications, elements of effective communication, listening skills, empathetic listening, role of perception in communication.

Assertiveness skills: the concept, assertiveness and self-esteem, advantages of being assertive, assertiveness and organizational effectiveness.

Self-perception and self-confidence: locus of control (internal v/s external), person perception, social perception, attribution theories-self presentation and impression management, the concept of self and self-confidence, how to develop self-confidence.

Goal setting: the concept, personal values and personal goals, goal setting theory, six areas of goal setting, process of goal setting: SMART goals, how to set personal goals

Time management: the value of time, setting goals/ planning and prioritizing, check the time killing habits, procrastination, tools for time management, rules for time management, strategies for effective time management

Presentation skills: the process of presentation, adult learning principles, preparation and planning, practice, delivery, effective use of voice and body language, effective use of audio visual aids, dos and don'ts of effective presentation

Public speaking-an art, language fluency, the domain expertise (Business GK, Current affairs), self-confidence, the audience, learning principles, body language, energy level and conviction, student presentations in teams of five with debriefing

Unit-2: Verbal (5 Lectures)

Vocabulary building: introduction to the methods and practices of learning vocabulary, learning through practice sets to face questions on antonyms, synonyms, spelling error, analogy, wrong form of words, frequently confused words, understanding the nuances of spelling changes and wrong use of words.

Grammar: Analyzing subject verb agreement, pronoun agreement, tense consistency, and misplaced or dangling modifiers, parallel construction, active and passive voices, faulty comparison

Students take a few online practice tests to understand the test taking strategy and work on their specific areas of improvement.

Unit-3: Aptitude (5 Lectures)

Introduction to numbers – number line, classification of numbers, prime and composite numbers, co-prime numbers, number of zeros in an expression, LCM, HCF, remainder theorem, rules of divisibility, base system

Basics of equations- introduction to simple and quadratic equations, roots of an equation, word problems, problems on ages, consistency of equations

Percentages, profit and loss: introduction to percentages, percentage change, value appreciation and depreciation, comparison observations, fundamentals concepts of business/commercial terminologies like cost price, selling price, profit, loss, marked price and discount

Ratio proportion and variation/partnership – fundamentals of ratios, duplicate ratio, triplicate ratio, sub duplicate ratio and sub triplicate ratio, direct and inverse proportion, joint variation, partnership and profit sharing

Averages and mixtures – mean, median and mode, measure of central tendency, concept of assumed average and weighted average, AM, GM and HM – relationship between AM, GM and HM, cheaper quantity and dearer quantity, rule of allegation, profit v/s quality of items getting mixed.

Simple interest and compound interest – time value of money, capital/principle, period of investment, rate of return, period of compounding, SAGR and CAGR

Data interpretation – representation of data using tables, bar charts, pie charts, case study, line graph, scatter diagram – analyzing the data for decision making

Venn diagrams- set theory – concept of sets, types of set, forms of set representation, power set, sub set and super set, 2 and 3 variable venn-diagrams, familiarity with words like AND, OR, atleast, atmost, exactly ‘n’ elements

Cubes – importance of aligning cuts to minimize/maximize the number of pieces of small cubes, painting a cube and cutting the cube, disintegration and integration of cubes, diagonal cutting, volume/LSA/TSA of cubes

References

- Andrew J DuRbin , “Applied Psychology: Individual and organizational effectiveness”, Pearson- Merril Prentice Hall, 2004
- Michael G Aamodt, “An Applied Approach, 6th edition”, Wadsworth Cengage Learning, 2010
- Robert Bolton, Dorothy Grover Bolton, “People Style at Work..and Beyond: Making Bad Relationships Good and Good”, Ridge Associates Inc., 2009
- John Hayes “Interpersonal skills at work”, Routledge, 2003
- Mark J Martinko, “Attribution theory: an organizational perspective”, St. Lucie, 1995
- Stephen Covey, “The habits of highly effective people”, Free press Revised edition, 2004
- Kenneth H Blanchard ,”The 25 Best Time Management Tools & Techniques: How to Get More Done Without Driving Yourself Crazy” , Peak Performance Press, 1st edition 2005
- S. Upendran, “Know Your English”, Universities Press (India) Limited, 2015

- Kaplan, “New GMAT Premier”, Kaplan Publishing, U.K., 2013
- Arun Sharma, “How to Prepare for Data Interpretation for the CAT Common Admission Test”, Tata Mc GrawHills, 3nd Edition, 2015
- R.S. Aggarwal, “A Modern Approach To Verbal & Non-Verbal Reasoning”, S. Chand Publishing, Revised -2015
- SarveshVerma, “Quantitative Aptitude-Quantum CAT”, Arihant Publications, 2016

22AVP103 Mastery Over Mind (MAOM) 1-0-2 2

Course Outcomes:

- Relate to the causes of stress in one’s life.
- Experiment with a range of relaxation techniques
- Model a meditative approach to work, study, and life.
- Develop appropriate practice of MA-OM technique that is effective in one’s life
- Inculcate a higher level of awareness and focus.
- Evaluate the impact of a meditation technique

1. Course Overview

Master Over the Mind (MAOM) is an Amrita initiative to implement schemes and organise university-wide programs to enhance health and wellbeing of all faculty, staff, and students (UN SDG -3). This program as part of our efforts for sustainable stress reduction gives an introduction to immediate and long-term benefits and equips every attendee to manage stressful emotions and anxiety facilitating inner peace and harmony.

With a meditation technique offered by Amrita Chancellor and world-renowned humanitarian and spiritual leader, Sri Mata Amritanandamayi Devi (Amma), this course has been planned to be offered to all students of all campuses of AMRITA, starting off with all first years, wherein one hour per week is completely dedicated for guided practical meditation session and one hour on the theory aspects of MAOM. The theory section comprises lecture hours within a structured syllabus and will include invited guest lecture series from eminent personalities from diverse fields of excellence. This course will enhance the understanding of experiential learning based on university’s mission: “Education for Life along with Education for Living”, and is aimed to allow learners to realize and rediscover the infinite potential of one’s true Being and the fulfilment of life’s goals.

2. Course Syllabus

Unit 1 (4 hours)

Causes of Stress: The problem of not being relaxed. Need for meditation -basics of stress management at home and workplace. Traditions and Culture. Principles of meditation– promote a sense of control and autonomy in the Universal Human Value System. Different stages of Meditation. Various Meditation Models. Various practices of Meditation techniques in different schools of philosophy and Indian Knowledge System.

Unit 2 (4 hours)

Improving work and study performance. Meditation in daily life. Cultivating compassion and good mental health with an attitude of openness and acceptance. Research and Science of Meditation: Significance of practising meditation and perspectives from diverse fields like science, medicine, technology. philosophy, culture, arts, management, sports, economics, healthcare, environment etc. The role of meditation for stress and anxiety reduction in one's life with insights based on recent cutting-edge technology. The effect of practicing meditation for the wholesome wellbeing of an individual.

Unit 3 (4 hours)

Communications: principles of conscious communication. Relationships and empathy: meditative approach in managing and maintaining better relationships in life during the interactions in the world, role of MAOM in developing compassion, empathy and responsibility, instilling interest, and orientation to humanitarian projects as a key to harness intelligence and compassion in youth. Methodologies to evaluate effective awareness and relaxation gained from meditation. Evaluating the global transformation through meditation by instilling human values which leads to service learning and compassion driven research.

TEXT BOOKS:

1.Mata Amritanandamayi Devi, "Cultivating Strength and vitality," published by Mata Amritanandamayi Math, Dec 2019
2.Swami Amritaswarupananda Puri ,"The Color of Rainbow " published by MAM, Amritapuri.

References:

1.Craig Groeschel, "Winning the War in Your Mind: Change Your Thinking, Change Your Life" Zondervan Publishers, February 2019
2.R Nagarathna et al, "New Perspectives in Stress Management "Swami Vivekananda Yoga Prakashana publications, Jan 1986
3. Swami Amritaswarupananda Puri "Awaken Children Vol 1, 5 and 7 - Dialogues with Amma on Meditation", August 2019
4. Swami Amritaswarupananda Puri "From Amma's Heart - Amma's answer to questions raised during world tours" March 2018
5. Secret of Inner Peace- Swami Ramakrishnananda Puri, Amrita Books, Jan 2018.

22NE681 Lab-I: Optoelectronics 0-0-4 -2

Pre-requisites: Basic understanding of experimental research

Total number of lab sessions: 15

Course Outcomes:

- *Students will be able to gain hands on experience in preparation and characterization of semiconductor nanomaterials.*
- *Practically correlate process parameters and property (electrical, optical…etc.)*
- *Fabricate devices and investigate their characteristics.*
- *Be able to learn operation of characterization tools and independently handle the instruments.*

- *A comprehensive experimental understanding of electrical and optical properties of semiconductors.*

Course Content:

Unit-1: Preparation and characterization of optoelectronic materials (4 sessions)

Synthesis of quantum dots by chemical method and size-property correlation. Metal-semiconductor junctions using PVD process. Characterization of nanomaterials.

Unit-2: Optical properties of materials and devices (5 sessions)

UV-VIS Spectroscopy, Optical reflectance and luminescence. Opto-electronic properties of bulk and thin films, LED characteristics.

Unit-3: Advanced semiconductors (3 sessions)

Nanoscale opto-electronics: advanced 2D materials processing and properties.

Unit-4: Standards in nanomaterials assessment and device testing (3 sessions)
Introduction to quality assessments, ISO, IEC standard testing.

TEXTBOOKS/ REFERENCES:
1. *S. M.Sze, "Physics of Semiconductor Devices", Wiley-Interscience, 1969.*
2. *D. K. Schroder, "Semiconductor Material and Device Characterization", 3rd Edition, Wiley Publishers, 2006.*

22NE682 Lab-II: Nanomaterials 0-0-4-2

Pre-requisites: Basic understanding of experimental research

Total number of lab sessions: 15

Course Outcomes:

- *Understand the preparation of standard solutions in different concentration units: Molarity, Molality and Normality*
- *Understand the synthesis of metal nanoparticles.*
- *Learn synthesis of plasmonic silver nanoparticles and observe its color change with varying size & shape of nanoparticles.*
- *Understand the principle and working of UV -Vis absorption spectroscopy technique and relation of absorption peak of silver nanoparticles with size and shape changes.*
- *Understand the synthesis of nanoparticles in non-aqueous route and observe its luminescence under UV lamp to understand quantum confinement effect.*
- *Understand the synthesis of nanoparticles in aqueous route and study the fluorescence properties of nanoparticles using spectrofluorometer*
- *Understand the UV-VIS absorption properties of nanoparticles and estimation of particle size using Brus equation*
- *Understand the principles of Atomic Force Microscope (AFM) and hands on experience in use of AFM in nanoparticle size characterization*
- *Understand the principles of Scanning Electron Microscope (SEM) and its use in characterizing nanoparticles*

Course Content:

Unit 1 (4 sessions)

Introduction to Nanolab and standard solution preparation, Synthesis of plasmonic silvernanoparticles *study its color change with varying size & shape of nanoparticles using UV -Vis absorption spectroscopy*

Unit 2 (5 sessions)

Preparation of metal oxide ZnO nanoparticles (Non-Aqueous route) and observe its luminescence under UV lamp, UV-VIS absorption properties of ZnO nanoparticles and estimation of particle size using Brus equation

Unit 3 (2 sessions)

Synthesis of Mn doped ZnS nanoparticles in aqueous route and study the fluorescence properties of nanoparticles using spectrofluorometer

Unit 4 (4 sessions)

Nanoparticle imaging for size and shape analysis using *Atomic Force Microscope (AFM) and Scanning Electron Microscope (SEM) characterizing nanoparticles*

References:

- *A Handbook of Laboratory Solutions, M H Gabb, Scientific Publishers, 2013*
- *Nanostructures & Nanomaterials: Synthesis, Properties & Applications; Guozhong Cao, Imperial College Press*

ELECTIVES (For Semester-1)

22NE631 Solid-State Phenomena at Nanoscale 3-0-0-3

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Understand the basics of crystal structure, lattice vibrations, Phonons*
- *Familiarize with the Harmonic oscillator model and Debye & Einstein models*
- *A thorough understanding of Dielectric, Ferroelectric and Piezoelectric concepts*
- *Gain in-depth knowledge in Magnetism & Superconductivity and understand its fundamental theories.*

Course content:

Unit 1. Chemical bonding and Crystal structures (10 lectures)

Solid state science: introduction to solids, materials classification by bonding, amorphous and crystalline materials, basics of crystal structure, lattice points and space lattice, Bravais

lattice, Lattice planes and Miller indices, the reciprocal lattice, bulk to Nano effects – examples, fundamental excitations on solids – brief (plasmons, polaritons and polarons).

Unit 2. Vibrations (8 lectures)

Lattice vibrations, a simple Harmonic oscillator, an infinite chain of atoms, the Brillouin zone, a finite chain of atoms, Modes of vibrations and density of states, Classical and quantum oscillator comparisons, Quantized vibrations-Phonons, Confinement of phonons (Nanoscale effects).

Unit 3. Thermal Properties (8 lectures)

Three-dimensional solids, Vibrational frequency estimation, Specific heat capacity, Classical theory and experimental results, Debye and Einstein models, Thermal conductivity, Anharmonic effects and thermal expansion, Heat Conduction.

Unit 4. Dielectrics, Ferroelectrics and Piezoelectrics (10 lectures)

Dielectric materials and phenomena, Microscopic Polarization, Frequency dependence of the Dielectric constant, Bulk, nano, thin-film dielectrics, High-K dielectrics and applications, Ferroelectrics and Piezoelectrics, Dielectric breakdown.

Unit 5. Magnetism and Superconductivity (10 lectures)

Magnetic effects in atoms, Diamagnetism, Magnons, paramagnetism, Curie and Pauli Paramagnetism, Ferromagnetic domains, Hysteresis, Nanoscale effects, Magnetic tunnel junctions, Magneto-resistance, Zero resistivity, The Meissner effect, BCS theory.

Textbooks:

1. *Solid-state Physics - An Introduction by P Hofmann, 2nd Edition, Wiley VCH (2015)*
2. *Introduction to Solid-State Physics by C. Kittel, 8th Edition, John Wiley and Sons (2005).*

22NE632 Quantum Science 3-0-0 (3 Credits)

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Understand the failure of classical mechanics*
- *Realize the importance of particle-like behavior of waves and wave-like behavior of particles.*
- *Understand initial success of quantization from blackbody radiation to Compton effect*
- *Know the importance of dual nature*
- *Distinguish the difference between classical models and Bohr's atom model and its success.*

- *Comprehensive understanding of Schrodinger's equation and its application to quantum systems.*

Course content:

Unit-1: Review of mechanics and failure of classical mechanics (10 lectures)

Review of mechanics, failures of classical mechanics,

Unit-2: Particle properties of waves (7 lectures)

Electromagnetic waves; blackbody radiation; Planck's quantum hypothesis, photo-electric effect, Compton Effect,

Unit-3: Wave properties of particles (7 lectures)

De Broglie waves; probability and phase and group velocities; particle in a box, wave-particle duality, uncertainty principle.

Unit-4: Atomic structure and models (6 lectures)

Atomic structure; atomic spectra; planetary model (classical); Bohr's H-atom model, Bohr's correspondence principle,

Unit-5: Schrodinger's equation and applications (15 lectures)

Wave equation; Schrodinger's equation (time dependent and independent), Linearity and superposition; expectation values; observables and operators; SE of particle in a box, finite potential well; harmonic oscillator; tunnelling.

TEXT BOOKS/REFERENCES:

1. Concepts of Modern Physics, A. Beiser, S. Mahajan and S. R. Choudhury 7th Edition, McGraw Hill, 2015
2. *Introductory Quantum Mechanics for Applied Nanotechnology by D. M. Kim, Wiley-VCH; 2015.*

22NE633 Modern Concepts in Materials Science 3-0-0 (3 Credits)

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Familiar with classification of materials and understand imperfections in solids.*
- *Understand diffusion, diffusion mechanisms and rate of diffusion.*
- *Will understand the importance of engineering materials such as, ferrous and non-ferrous alloys, ceramics and polymers.*
- *Get introduced to materials relevant thermodynamics and kinetics.*
- *To be able to recognize different mode of failure for materials and their testing.*

Course Content:

Unit-1: Introduction to materials and imperfections (10 lectures)

Types of materials; Crystalline and amorphous materials, imperfections in solids: dislocations, point defects, surface defects; structure-property correlations.

Unit-2: Atomic movements (8 lectures)

Introduction to diffusion; diffusion mechanisms; activation energy; rate of diffusion; Fick's laws of diffusion.

Unit-3: Engineering materials (7 lectures)

Alloys; ferrous alloys and non-ferrous alloys; ceramics (example: glasses and their applications); polymers and their applications.

Unit-4: Thermodynamics and kinetics of materials (10 lectures)

The thermodynamics aspect includes laws of thermodynamics, solution theory and equilibrium diagrams. The kinetics aspect includes diffusion, phase transformations, and the development of microstructure.

Unit-5: Failure of materials (10 lectures)

Corrosion (chemical and electrochemical); oxidation and other gas reaction; wear and erosion; fracture in metals and non-metals; non-destructive testing.

TEXT BOOK/REFERENCES:

1. *The Science and Engineering of Materials by Donald R. Askeland, Wendelin J. Wright, Cengage learning (2015).*

22NE611 Nano Engineering Applications 2 0 1 3

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *To understand the basics of energy conversion and storage at nanoscale (phenomena to devices)*
- *Introduce the fabrication and characterization technologies of Solar cells, batteries, thermo-electric and piezo-electric devices.*
- *Applications of electrochemical analysis techniques in characterizing energy storage devices*

Course Content:

Unit 1: Concepts in Energy conversion (8 lectures)

Semiconductor junctions, Shockley–Queisser limit, electrical and optical characteristics; Energy conversion at nanoscale, charge carrier dynamics at nanoscale in energy conversion devices

Unit 2: Energy conversion devices (12 lectures)

Solar cells: I-V, EQE, CV, and VOC decay, wafer, thin films and excitonic solar cells; carrier transport and loss mechanisms, recombination models; anti-reflective coating, surface texturing; photodetectors and LEDs.

Unit 3: Thermo-electric and piezo-electric devices (8 Lectures)

Thermo-electric and piezo-electric materials and devices, fabrication and characterizations.

Unit 4: Energy storage devices (10 Lectures)

Positive and negative electrodes of batteries and electrochemical capacitors, advanced batteries with nanoscale materials, Reaction mechanisms and fundamental understanding, cycle-life, capacity, energy and power density assessments, safety concerns and solutions.

Unit 5: Electrochemical analysis techniques (8 Lectures)

Electrochemical methods: potentiostatic and galvanostatic, cyclic voltammetry, chronoamperometry, chronopotentiometry and electrochemical impedance spectroscopy.

TEXT BOOKS/REFERENCES:

1. Jenny Nelson, "The Physics of Solar Cells", First Edition, Imperial College Press, 2003.
2. Stephen Fonash, Solar Cell Device Physics - 2nd Edition, Academic Press, 2010
3. L. R. Martinez and N. Omar, Emerging Nanotechnologies in Rechargeable Energy Storage Systems, 1st Edition, Elsevier (2017).
4. G. A. Nazri and G. Pistoia, Lithium Batteries, Springer, 2009.
5. Allen Bard and Larry R. Faulkner, Electrochemical Methods, John Wiley & Sons Inc, 2001.

22NE612 VLSI Technology and Design 3-0-0 (3 Credits)

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Introduced to wafer level fabrication and packaging.*
- *To be able to understand the design of logical circuits, operation and testing.*
- *Know the role of circuit elements including generators, detectors, comparators and counters, multipliers and shifters.*
- *Distinguish types of ASICs and arrays.*
- *Introduced to design software and packages utilized in the industry.*

Course Content:

Unit-1: Fabrication and proceses

Introduction to wafer fabrication, Packaging, MOS process (n-well and p-well), Silicon on insulator process.

Unit-2: VLSI design and testing

Introduction to VLSI Design, Basic MOS transistors, Enhancement mode transistor operation, Drain current Vs voltage derivation, NMOS and CMOS inverters, Sheet Resistance and capacitance, Delay, Driving large Capacitive Loads, Propagation delay, Fan-in and fan-out characteristics, introduction to scaling.

Unit-3: Circuit elements

Alternative CMOS Logic structures, Design of Adders, Parity generators, Detectors, Comparators and Counters, ALU, Multipliers and Shifters, memory elements.

Unit-4: Arrays

Types of ASICs, Standard Cell Array, Gate Arrays, Programmable Array Logic- PLAs, CPLDs, FPGAs,

Unit-5: Design software and packages

Design capture and verification tools, preparation and testing. Industrial relevant software packages (ex: Cadence, Ansys, CAD…etc.)

TEXT BOOKS / REFERENCES:

1. *Kamran Eshraghian, Eshraghian Dougles and A. Pucknell," Essentials of VLSI circuits and systems", PHI, 2005 Edition.*
2. *CMOS VLSI Design: A Circuits and Systems Perspective by Neil Weste and David Harris (2010) Pearson; 4th edition.*

22NE683 Lab-III: Nanoelectronics and Nanofabrication 0-0-4-2

Pre-requisites: Basic understanding of experimental research

Total number of lab sessions: 15

Course Outcomes:

- *Electronic transport characterization of nanomaterials with hands on experience.*
- *Will be trained to use cryogenic systems and materials characterization at low and high temperatures.*
- *Will be able to handle Laser based lithography systems to design nanoscale devices in the clean room environment.*
- *PCB design and fabrication will be explored.*

Course Content:

Unit-1: Electronic transport in nanoscale and cryogenics (5 sessions)

Hands of experiments involving electronic transport in nanoscale materials (quantum dots, nanowires, carbon nanotubes), low temperature and high temperature measurements.

Unit-2: Nanofabrication and characterization (5 sessions)

Lithography process and device fabrication, ensemble and isolated nanostructures electrical and photonic characterizations.

Unit-3: PCB design and cleanroom usage training (5 sessions)

PCB design and fabrication (ex: design using EsayEDA or similar platform). Exposure to cleanroom protocols and usage.

22NE684 Nano Energy Devices Lab 0-0-4 -2

Pre-requisites: Basic understanding of experimental research

Total number of lab sessions: 15

Course Outcomes:

- *Hands on experience in energy conversion devices: fabrication and testing.*
- *In depth exposure to energy storage materials and devices: fabrication and testing.*

Course Content:

Unit-1: Energy conversion devices (7 sessions)

Dye sensitized solar cell fabrication and testing, thin film hetero-junction photovoltaic device fabrication and testing, Quantum dot solar cell fabrication and testing,

Unit-2: Energy storage devices (7 sessions)

Li ion battery anode and cathode half-cell fabrication and testing, Li ion battery full-cell fabrication and testing, Supercapacitor/Pseudocapacitor fabrication and testing.

22NE613 Ethics in Research and Research Methodology 1 0 1 2

Pre-requisites: Any undergraduate degree

Total number of classes: 30

Course Outcomes:

- *Understand the basic concepts of ethics in proper conduct of research*
- *Understand about plagiarism in research and how it should be avoided*
- *Gain a clear idea about the importance of proper data documentation*
- *Students will have a clear idea about the research methodologies that need to be adopted during their research*

Course Content:

Unit-1 (15 Lectures)

Plagiarism, regulatory principles, safety in research, ethics in nanomaterials based research.

Unit-2 (15 Lectures)

Principles of data documentation, protocol development, research questions and hypothesis driven research.

TEXTBOOKS:

1. *Research Ethics for Scientists, C. Neal Stewart Jr., Wiley-Backwell Publishers, 2011*
2. *Ethics in Science, Ethical Misconduct in Scientific Research, John D'Angelo, CRC Press, 2012*

ELECTIVES (For Semester-2)

22NE641 Emerging Nano-manufacturing technologies 3-0-0

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Introduced to vacuum techniques (how to create and measure vacuum).*
- *Deeper understanding of physical vapour deposition techniques.*
- *Fundamental exposure of chemical vapour deposition.*
- *Theoretical understanding of advances in nanofabrication techniques*
- *Explore nanomaterials based device fabrication techniques and advanced manufacturing processes.*

Course Content:

Unit-1: Thin-films deposition by vacuum and non-vacuum processes (18 lectures)
Vacuum science and technology, physical vapour deposition: process and systems, thermal evaporation, electron beam evaporation, sputtering (DC, RF magnetron) chemical vapour deposition, film formation and nanostructure, characterization of thin films.

Unit-2: Advanced micro and nanofabrication techniques (12 lectures)
Micro- and nanofabrication overview, Photolithography, e-beam lithography. Modern fabrication technologies: nano-imprint lithography, soft lithography, microfluidic applications and devices.

Unit-3: Device fabrication and advanced processing methods (15 lectures)
Fabrication of 0 to 2-D nanostructures, Transistors and electronic building blocks, MEMS/NEMS, Applications of nanofabrication. Additive manufacturing and variants of 3D printing (electrochemical, laser sintering, jet fusion…).

TEXT BOOKS/REFERENCES:

1. *Z. Cui, Nanofabrications: Principles, capabilities and limits, Springer (2017).*
2. *T. Li and Z. Liu, Outlook and challenges in Nanodevices, Sensors and MEMS, Springer (2017).*
3. *Handbook of Thin Film Technology, H. Frey and H. R. Khan, Springer Science and Business Media (2015)*
4. *The Materials Science of Thin Films, Milton Ohring, Academic Press (2002).*
5. *Additive Manufacturing by C.P. Paul, A.N. Jinoop, McGraw Hill (2021).*

22NE642 **Polymeric Nanomaterials** **3-0-0**

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *To understand the basic concept of polymer science, polymer synthesis and preparation techniques.*
- *Learn about characterization and thermal properties of polymeric materials.*
- *To understand about biopolymer composites degradable and non-degradable polymers, hydrogel, dendrimers, hydrogels and thermos-sensitive polymers.*
- *Learn about the different type of polymeric nanomaterials fabrication and their applications in biomedical field.*

Course Content:

Unit-1 (15 lectures)

Introduction and Basic Concepts of Polymer Science-Classification of polymers, polymer properties, Polymer synthesis, chain polymerization–mechanism of free radical, cationic, anionic and co-ordination polymerization–ring opening polymerization-Copolymerization-preparation of block and graft copolymers, cross-linked polymers, conductive polymers and their composites.

Unit-2 (15 lectures)

Techniques of polymerization–bulk, solution, emulsion, suspension, interfacial, gas phase and melt polycondensation and Determination polymer molecular weight and size. Thermal properties of polymers-Glassy and Rubbery state, glass transition temperature, Factors affecting Tg and crystallinity of polymers, Determination of Tg and Tm – polymer characterization – TGA, DTA and DSC of polymers.

Unit-3 (15 lectures)

Natural and Synthetic biopolymers; Biopolymer composites-both degradable and non-degradable; Dendrimers-Structure, Preparation; Types of hydrogels, in situ/injectable hydrogels, thermo-sensitive polymers-LCST properties. Polymeric nanoparticles and nanogel-preparation methods; Different types Nanofibers and nanocomposite scaffolds preparations. Biomedical applications of nanoparticles, nanogels, nanofibers and nanocomposite scaffolds.

Text book/References

1. *V. R. Gowariker, N. V. Viswanathan and JayadevSreedhar, "Polymer Science" New Age International (p) Ltd., New Delhi, 2015.*
2. *Michael Niaounakis, "Biopolymers: Applications and Trends", 1st Edition, Elsevier, 2015.*
3. *Challa S. S. R. Kumar, "Polymeric Nanomaterials", Wiley, 2011.*

22NE643 Nanophotonics 3-0-0

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Understand how the light-matter interactions are depends on particle size (bulk to nanoscale)*
- *Be familiar with Near-field optics and localized surface plasmons*
- *Understand the use of photonic crystals as a waveguides*
- *Learn optical metamaterials and its application in imaging the objects.*
- *Comprehend the working of nanolasers and Quantum cascade lasers.*

Course Content:

Unit 1: Introduction (10 lectures)

Review of vector analysis, Electrostatics, Electric fields in matter, Magnetostatics, Magnetic field in matter, introduction to Nanophotonics.

Unit 2: Basics of nanophotonics (7 Lectures)

Photons and electrons: similarities and differences, free-space propagation, Confinement of photons and electrons. Localization under a periodic potential: Bandgap, Cooperative effects. Nanoscale optical interactions, Nanoscale confinement of electronic interactions.

Unit 3: Near-field optics and microscopy (8 Lectures)

Electrodynamics, light-matter interactions, concepts and devices in nanoscale optics and photonics. Nano-scale and near-field optics, near-field optical probes, near-field scanning optical microscopy, transmission through nanoscale apertures.

Unit 4: Lasers and quantum lasers (8 Lectures)

Solid-state lasers and gas lasers, Quantum materials, Quantum confined structures as lasing media, nanolasers, Quantum Cascade Lasers.

Unit 5: Plasmonics and photonic crystals (12 Lectures)

Metallic Nanoparticles and Nanorods, Local field enhancement, Plasmonic wave guiding, Applications of metallic nanostructures, Photonic crystals (0D, 1D, 2D & 3D), silicon, graphene and diamond photonics, metamaterials, single-photon sources.

TEXT BOOKS / REFERENCES:

1. *J. W. Haus, "Fundamentals and Applications of Nanophotonics", Woodhead Publishing, 2016.*
2. *S. V. Gaponenko, "Introduction to Nanophotonics", Cambridge University Press, 2010.*
3. *Introduction to Electrodynamics, David J Griffiths, 3rd edition, 1999.*

22NE644 Digital Electronics 3-0-0-3

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Understand the concepts and laws of combinational and sequential logic circuits*
- *Design the combinational logic circuits*
- *Gain the knowledge of how to design the sequential circuits using RS, JK, T flip-flops*
- *Learn applying the designs of combinational and sequential circuits in microprocessors and microcontrollers.*

Course Content:

Unit 1: Number systems and Binary codes (10 lectures)

Analog and digital number systems (decimal and binary), Deci-Binary, Binary-Deci, Hexa-Deci conversion, rules of binary addition, subtraction, multiplication and division,

Unit 2: Logic gates and related devices (8 lectures)

Positive and negative Logic, Truth table, Logic gates (AND, OR, NOT, NAND, NOR….), Universal gates, Universal gates

Unit 3: Logic Families (10 Lectures)

Introduction to transistor-transistor logic (TTL), CMOS logic family, NMOS and PMOS Logic, Boolean algebra, variables, literals and terms in Boolean expressions, Postulates and theorems of Boolean Algebra.

Unit 4: Flip-flops and its applications (8 lectures)

Multivibrator, Integrated circuit (IC) multivibrator, *R*-S Flip-flops, J-K Flip-flop, T Flip-flop.

Unit 5: Applications of Digital circuits (10 lectures)

Counters and converters, Ripple counter, Synchronus counter, Modulus of a counter, Decoding/cascading counter, Digital-to-Analogue converter, microprocessors and microcontrollers, memory devices.

TEXT BOOKS / REFERENCES:

1. *Digital Electronics: Principles and Integrated Circuits by AK. Maini, Wiley (2007).*
2. *Microprocessor Architecture- Programming and Application with 8085" by R S Gaonker, Wiley Easter (2013).*
3. *Modern Digital Electronics by RP Jain, McGraw HIll (2010).*

ELECTIVES (For Semester-3)

22NE731 Nanocarbon and Nanocomposites 3-0-0-3

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *Understand how to synthesize and characterize the carbon based nanostructures*
- *Gain knowledge on nanocomposites and its applications*
- *Be familiar with structural, electrical and electrochemical properties of Carbon nanocomposites*
- *Learn the synthesis and design strategies of metal organic frameworks*

Course Content:

Unit 1: Carbon Nanostructures (10 Lectures)

Introduction to carbon and its nanostructures, graphite, single walled and multi-walled carbon nanotubes, fullerenes, graphene, graphene oxide, amorphous nanocarbon.

Unit 2: Properties of Carbon Nanomaterials (12 Lectures)

Structure, size, synthesis, optical and mechanical properties; applications in nanoelectronics, energy conversion and energy storage.

Unit 3: Carbon nanocomposites (12 Lectures)

Metal/Carbon nanocomposites, Nanocomposites of carbon with other inorganic materials and its applications.

Unit 4: Organic frameworks (10 Lectures)

Organic frameworks of nano-materials (including MOF and COF) design strategies, synthesis, characterization and their application in nanoelectronics and energy.

TEXT BOOKS/REFERENCES:

1. *Carbon Nanotechnology: Recent developments in chemistry, physics, materials science and device applications edited by Liming Dai, Elsevier-2006.*
2. *Carbon Nanomaterials: Synthesis, Structure, Properties and Applications by Rakesh B. Mathur, B.P.Singh and S. Pande, CRC Press-2017*
3. *Introduction to Reticular Chemistry: Metal-Organic Frameworks and Covalent Organic Frameworks by O.M. Yaghi, M.J. Kalmutzki and C.S. Diercks, Wiley-2019*

22NE732 Nanosensors 3-0-0-3

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 45

Course Outcomes:

- *To understand the fundamentals of sensing devices.*
- *To develop an understanding about the various components of a sensor and its fabrication.*
- *To comprehend the mechanisms of sensing.*
- *To understand the classifications of sensors based on the mechanism used.*
- *Recent advances in sensors and how nanotechnology facilitates easier sensing.*

Course Content:

Unit-1 (8 lectures)

Introduction to sensors and nanosensors; transducers and actuators; classification of sensors; characteristics of sensors; active and passive sensors; contact and non-contact sensors; absolute and relative sensors;

Unit-2 (15 lectures)

Mechanisms of sensing, Optical; chemical; physical sensors; Gas sensors; mass sensors; thermal sensors; Fabrication and testing. Comparison of bulk and nano effects in sensing

Unit-3 (10 lectures)

Nano-electromechanical sensors; electrochemical sensors; working principles; fabrication and testing; Introduction to biosensors; bio-chemical sensors; sensors in medical applications; lab on chip;

Unit-4 (10 lectures)

Nanomaterial based large scale sensors; miniaturized sensors; Recent advances in sensors (ex: wearable sensors)

Review (2 lectures)

References

1. *Craig Grimes, Elizabeth Dickey, Michael Pishko, "Encyclopedia of Sensors" American*
2. *Scientific Publishers, 2006.*
3. *Sandra Carrara, Nano-Bio-Sensing, Springer, New York, 2011, ISBN: 978-1-4419-6169-3.*
4. *Francisco J. Arregui, Sensors based on nanostructured materials, First Edition,*
5. *SpringerVerlag, New York, 2009, ISBN: 978-0-387-77752-8.*

22NE733 Computational Methods for Condensed Matter 3 0 0 3

Pre-requisites: Basic math, physics and chemistry

Total number of classes: 30 + 7 Lab sessions

Course Outcomes:

- *Introduced to fundaments of computation relevant for condensed matter physics.*
- *Understanding first principles calculations of materials.*
- *Introduced to simulations using Monte Carlo and molecular dynamics.*
- *Practical hands on training in computational tools for physical and chemical property calculation of materials.*

Course Content:

Unit-1: Fundamentals of condensed matter computation (15 lectures)

Interatomic potentials or force fields, structure chemistry and properties relations, first-principle based density functional atomic simulations methods, pseudopotentials, total energy functional and its derivatives, boundary conditions for molecules, clusters and extended systems, Ewald simulation using classical potentials.

Unit-2: Properties and simulations (15 lectures)

Vibrational principles, methods of optimization for linear problem and nonlinear problems. Errors and accuracy of quantitative predictions: thermodynamics ensembles, Monte Carlo sampling, molecular dynamics simulation. Free energy and phase transitions. Fluctuations, Susceptibilities and transport properties. Couse-graining approaches and mesoscale models.

Unit-3: Hands on Computational training (7 sessions)

This course offers a project involving simulations for physical or chemical properties of a material of student's choice (for 1 credit). Introduction to multi-physics software such as Matlab, Comsol…etc.

TEXTBOOKS/ REFERENCES:

1. *Electronic structure: Basic Theory and Practical Methods, by Richard Martin Cambridge University Press (2004).*
2. *Computer Simulations of Liquids by M.P. Allen and D. J. Tildesley, Oxford Scholarship (2017).*
3. *www.electronicstructure.org*
4. *Understanding Molecular Simulations by D. Frenkel and B. Smit, Academic Press (2002)*

22NE798 Dissertation – Mini project 0-0-20 (10 Credits)

22NE799 Dissertation – Project 0-0-32 (16 Credits)

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