

# SYLLABUS

## 19MA617 MATHEMATICAL FOUNDATIONS FOR MATERIALS SCIENCE 3-0-0-3

Mathematical representation of problems – Vector & Matrix Algebra: Vector spaces, Linear independence, Basis of a space, Basics of Matrix Algebra, Eigenvalues & Eigenvectors; Basics of Numerical Analysis: Error analysis, Computations of errors of algorithms, Stiffness of algorithms, Interpolation (Lagrange approximation), Polynomial approximation and curve fitting (Newton method), Numerical differentiation and integration (Trapezoidal and Simpson's rules); Linear Algebraic Equations:  $Ax = b$  (Gauss-Jordan and Gauss-Seidel), Numerical techniques for ODEs (Euler method, Runge-Kutta method); Partial Differential Equations: Numerical techniques for parabolic and elliptic equations – finite differences

**TEXT BOOKS/REFERENCES:**

1. A. K. Ray and S. K. Gupta, *Mathematical Methods in Chemical and Environmental Engineering*, Second Edition, Cengage Learning Asia, 2003.
2. E. Kreyszig, *Advanced Engineering Mathematics*, Ninth Edition, John Wiley & Sons, 2006.
3. V. G. Jenson and G. V. Jeffreys, *Mathematical Methods in Chemical Engineering*, Second Edition, Academic Press, San Diego, 1978.
4. M. K. Jain, S. R. K. Iyengar and R. K. Jain, *Numerical Methods for Scientific and Engineering Computation*, Fifth Edition, New Age International, New Delhi, 2008.
5. P. Ahuja, *Introduction to Numerical Methods in Chemical Engineering*, Prentice Hall India, 2010

CO Code	Course outcome statement
19MSE601.1	Be able to formulate mathematical problems and identify the correct numerical methods for solving them
19MSE601.2	Represent systems in terms of linear algebraic equations (scalar and vector) and understanding the methodology of solving them, for material and conceptual reconciliation in physical systems
19MSE601.3	Understand and apply techniques of curve-fitting and interpolation, to aid in mathematical modelling of relationships in coordinate data
19MSE601.4	Identify systems where numerical differentiation and integration are required, and apply suitable methods for the same
19MSE601.5	Understand and apply numerical methods for solving ordinary and partial differential equations, for physical rate-change systems
19MSE601.6	Understand impact of measurement error, and apply methods for assessment of measurement variation for a given system

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
---------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------

19MSE601.1	3	3	3	3	3				2	1	1	2
19MSE601.2	3	3	3	3	3				2	1		1
19MSE601.3	3	3	3	3	3				2	1	2	1
19MSE601.4	3	3	3	3	3				2	1	2	1
19MSE601.5	3	3	3	3	3				2	1	2	1
19MSE601.6	3	3	3	3	3				2	1		2

### 19MS601

### ENGINEERING MATERIALS

3-0-0-3

Classification of Engineering Materials: Metals, Ceramics, Polymers, Composites and Their Types; Material Structure, Bonding, Crystals: Lattice, Points, Directions, Planes – Miller Indices, Reciprocal Lattice, Crystal Systems and Bravais Lattices, Primitive and Non-primitive Cells; Crystal Defects: Point Defects, Frenkel and Schottky Defects, Line and Planar Defects, Grain Boundaries; Diffusion in Solids: Fick's 1<sup>st</sup> and 2<sup>nd</sup> laws, Ideal solutions, Kirkendall Effect, Darken's Analysis, Estimation of Diffusion Coefficient; Solid Solutions, Intermetallics; Cooling Curves and Phase Diagrams: Isomorphous and Eutectic Phase Diagrams; Iron-Carbon Phase Diagram: Cast Iron and Steels; Phase Diagrams of Non-Ferrous Metals & Alloys

#### TEXT BOOKS/REFERENCES:

1. W. D. Callister, Jr., “*Materials Science and Engineering*”, Sixth Edition, Wiley India, 2003.
2. W. F. Smith, J. Hashemi and R. Prakash, “*Materials Science and Engineering*”, Fourth Edition, Tata Mc Graw Hill, 2008.
3. D. Askeland, P. Fulay, W. J. Wright and K. Balani, “*The Science and Engineering of Materials*”, Sixth Edition, Cengage, 2012.
4. S. H. Avner, “*Introduction to Physical Metallurgy*”, Second Edition, McGraw Hill, 1997.
5. V. Raghavan, “*Materials Science and Engineering: A First Course*”, Fifth Edition, Prentice Hall India, 2004.

CO Code	Course outcome statement
19MS601.1	Understand various types of engineering materials used in the industrial and domestic applications
19MS601.2	Study the crystal structure, defects, grain boundary and diffusion effects in ceramics and semiconductors; the conformations, properties of various polymers and composites
19MS601.3	Analyze the phase diagrams, heat treatment methods, structure and properties of metals and metal alloys

19MS601.4	Design and preparation of engineering materials with desirable properties for performance improvements in systems and devices
-----------	---

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS601.1	3	1	2	2	1	1	1					
19MS601.2	2	2	2	3	3	1						
19MS601.3	2	2	2	3	3	1						
19MS601.4	2	2	3	3	3	1	1					

## 19MS602

## MATERIALS THERMODYNAMICS

## 3-1-0-4

Entropy – Statistical Meaning; Combined First and Second Laws; Physical Meaning of Entropy, Pressure, and Chemical Potential; Postulational Approach to Thermodynamics: Criteria for Thermodynamic Equilibrium, Euler and Gibbs-Duhem Equations, Phase Rule, Thermodynamic Potentials, and Criteria for Stability; Solid Equilibria; Mixtures and Solutions: Raoult's and Henry's Laws; Gibbs Free Energy of Solution; Activity Coefficients and Models; Regular Solutions, Criteria for Phase Stability; Phase Diagrams; Reactions involving Pure Condensed Phases - Ellingham Diagrams, Effects of Phase Transformations; Phase Diagrams of Binary Systems - Isomorphous, Eutectic, and Peritectic Systems; Disorder-to-order transformations, ordered alloys, thermodynamics of point defects, surfaces, and interfaces, Glass science; First-order and other transitions; Amorphous and Glassy materials; Thermodynamics of Nucleation; Stability

### TEXTBOOKS/REFERENCES:

1. D. R. Gaskell, “*Introduction to the Thermodynamics of Materials*”, Fifth Edition, Taylor & Francis, New York, 2008
2. A. Ghosh, “*Textbook of Materials and Metallurgical Thermodynamics*”, Prentice Hall India, 2002.
3. Y. A. Cengel and M. A. Boles, “*Thermodynamics: An Engineering Approach*”, Seventh Edition, Tata McGraw Hill, 2011.
4. Y.V.C. Rao, “*Chemical Engineering Thermodynamics*”, Universities Press, New Delhi, 1997.
5. J. P. O'Connell and J. M. Haile, “*Thermodynamics: Fundamentals for Applications*”, Cambridge University Press, 2005.

CO Code	Course outcome statement
---------	--------------------------

19MS602.1	Understand the fundamentals of thermodynamics, energy & entropy, heat & work, processes, equilibrium and phase change
19MS602.2	Understand the fundamentals of ideal solutions, real solutions and origin of miscibility gap.
19MS602.3	Understand the origin of isomorphous and eutectic phase diagrams and apply them in manufacturing processes
19MS602.4	Understand thermodynamic necessity for existence of defects, predict defect formation and understand disorder-to-order transformations
19MS602.5	Understand the nucleation process and differentiate the homogeneous nucleation and heterogeneous nucleation in terms of free energy and kinetics.

CO Code	PO 1	PO 2	PO 3	PO 4	PO5	PO 6	PO 7	PO8	PO 9	PO 10	PO 11	PO 12
19MS602.1	3	3	2	2					2	1		1
19MS602.2	3	3	3	2	1				2	1		1
19MS602.3	3	3	3	3	1				2	1		1
19MS602.4	3	3	3	3	1				2	1		1
19MS602.5	3	3	3	3	1				2	1		1

### 19MS603

### ELECTRONIC MATERIALS SCIENCE

4-0-0-4

Electrical Conduction in Solids – Metals, Semiconductors, Ionic Solids; Drude Model, Factors Affecting Resistivity: Temperature and Impurities, Alloys, Mattheissen and Nordheim Rules, Resistivities of Mixed Solid Phases, Hall Effect; Basic Quantum Physics – Atomic Structure, Molecular Orbital Theory, Band Theory and Occupation Statistics in Metals and Non-Metals; Fermi Level; Conductivity of Metals; Metal-Metal Junction: Contact Potential, Seebeck and Peltier Effects; Thermocouples; Intrinsic and Extrinsic Semiconductors; Temperature Dependence of Conductivity; Recombination and Trapping; Drift and Diffusion Currents; Working of Semiconductor Devices using Band Diagrams and their Electrical Characteristics: *pn* junctions, Forward and Reverse Bias, BJT, MOSFET; Dielectric Properties of Materials: Polarization and Permittivity, Mechanisms of Polarization, Dielectric Properties – Dielectric Constant, Dielectric Loss, Dielectric Strength and Breakdown, Piezoelectricity, Ferroelectricity, and Pyroelectricity; Magnetic properties and Superconductivity: Magnetic moments and Magnetic Permeability, Types of magnetism, Saturation

magnetization, Magnetic domains, Soft and Hard Magnetic Materials, Superconductivity and its Origin, Giant Magneto Resistance, Josephson effect, Applications – Magnetic Recording; Optical Properties of Materials: Reflection, Refraction, Dispersion, Refractive Index, Snells Law, Light Absorption and Emission, Light Scattering, Luminescence, Polarization, Anisotropy, Birefringence; Optoelectronic Properties of Materials and Optoelectronic Devices: LEDs, Solar Cells, Lasers, pin diodes, photodiodes; Thermal Properties of Materials: Heat Capacity, Thermal Expansion, Thermal Conductivity, Thermal Stresses

#### TEXTBOOKS/REFERENCES:

1. S. O. Kasap, “*Principles of Electronic Materials and Devices*”, 2006, Third Edition, Tata McGraw Hill.
2. W. D. Callister, Jr., “*Materials Science and Engineering*”, 2006, Sixth Edition, Wiley India.
3. D. Jiles, “*Introduction to the Electronic Properties of Materials*”, Chapman & Hall. 1994.

CO Code	Course outcome statement
19MS603.1	Understand the mechanisms and models of electrical and thermal conduction in metals semiconductors and dielectrics based on classical and quantum models
19MS603.2	Apply the classical and quantum models to junctions involving metals, insulators and semiconductors, understand device designs and predict performance
19MS603.3	Understand the origin of polarization in dielectric materials, piezoelectricity, ferroelectricity and pyroelectricity, and apply the classical and quantum models to predict polarization
19MS603.4	Understand the origin of magnetism and magnetic properties of materials, and analyse their behaviour in different applications
19MS603.5	Understand optical properties of materials and analyse their application in optoelectronic devices

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS603.1	3	3	3	2					2	1		1

19MS603.2	3	3	3	3					2	1		1
19MS603.3	3	3	3	3					2	1		1
19MS603.4	3	3	3	3					2	1		1
19MS603.5	3	3	3	3					2	1		1

## 19MS604

## STATISTICAL DESIGN OF EXPERIMENTS

2-1-0-3

Introduction to the role of experimental design; basic statistical concepts; sampling and sampling distribution; Testing of hypotheses about differences in means - randomized designs and paired comparison designs; testing of hypotheses about variances; Analysis of variance (ANOVA) – oneway classification ANOVA; analysis of fixed effects model; comparison of individual treatment means; the random effects model; the randomized complete block design; Principle of Least Squares and Linear Regression; Model assumptions and residual analysis;  $2^k$  Factorial and Fractional Factorial Designs (Plackett-Burman); concepts of coded & un-coded variables, repetition, replication, and randomization; graphical and numerical analysis; concepts of confounding and orthogonal contrasts; model interpretation, checking of model assumptions, predictions, and simultaneous optimization; Split-plot designs; Response Surface Methodology – central composite designs (structure, rotatability, orthogonality, types of CCD, analysis); Box-Behnken designs; Mixture designs - structure, analysis, and applications; Basics of Taguchi designs

### TEXTBOOKS/REFERENCES:

1. D. C. Montgomery, “*Design and Analysis of Experiments*”, Sixth edition. New York, New York: John Wiley & Sons, 2005.
2. Box, Hunter, and Hunter, “*Statistics for Experiments*”, Second edition. Wiley-Interscience, 2005.
3. J. Antony, “*Design of Experiments for Engineers & Scientists*”, Butterworth-Heinemann, 2003.
4. Z. Lazic, “*Design of Experiments in Chemical Engineering*”. Wiley-VCH, Weinheim, 2004.

CO Code	Course outcome statement
19MS604.1	Understand the role of statistics in experimental research, and apply numerical methods for descriptive and graphical representation of data
19MS604.2	Understand and apply concepts of probability distributions for modeling variation in sampling statistics
19MS604.3	Formulate and test statistical hypothesis on population mean, variance, and proportion to aid in answering research questions

19MS604.4	Understand the theory of statistical design of experiments, and create designs for real-world research questions
19MS604.5	Apply concepts of hypothesis testing and linear regression to analyze experimental data from different types of designs (factorial, response surface, and mixture)

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS604.1	3	3	1	1	2							
19MS604.2	2	1	1	1	2							
19MS604.3	3	2	1	2	2							
19MS604.4	3	2	3	3	3							
19MS604.5	2	2	3	3	3							

## 19MS605 MATERIALS PROCESSING

4-0-0-4

### Metals and Alloys

Metal casting; forming and shaping processes: rolling, forging, extrusion, drawing, sheet and metal forming; joining processes: welding, machining; Powder metallurgy: pressing and sintering; Drilling, milling, cutting; grinding

### Ceramics

Glass working; Processing of traditional, new ceramics and cermets; powder pressing, tape casting

### Polymers

Polymerisation: Condensation, Addition, Bulk, Solution, Suspension, Emulsion; Polymer Processing: Mixing, extrusion, moulding, spinning, casting, calendaring, joining, foam processing, rubber processing, and machining of plastics, processing of polymer matrix composites, solvent cementing, adhesive bonding

### Nanomaterials

Top-down and bottom-up approach; optical and E-beam lithography, MBE, etching, vacuum processing/PVD and CVD; molecular self-assembly; nanoparticle synthesis – sol gel, solid phase, solvothermal and co-precipitation processes

### TEXTBOOKS/REFERENCES:

1. S. Kalpakjian and S. R. Schmid, “*Manufacturing Engineering and Technology*”, Fourth Edition, Pearson Education India, 2002.
2. M. P. Groover, “*Principles of Modern Manufacturing*”, Fifth Edition, SI Version, Wiley India, 2014.
3. M. D. Ventra, S. Evoy and J. R. Heflin, “*Introduction to Nanoscale Science and Technology*”, Kluwer Academic Publishers, 2004.
4. Chanda and S. K. Roy, “*Plastics Technology Handbook*”, CRC Press, Atlanta, 2007.
5. A. Ghosh and A.K. Mallik, “*Manufacturing Science*”, Affiliated East-West Press Pvt. Ltd., 2010.

CO Code	Course outcome statement
19MS605.1	Appreciate the forming, shaping, and joining processes employed for metallic materials
19MS605.2	Identify the various processes for the manufacture of ceramic products..
19MS605.3	Classify different polymerization processes and comprehend various plastics conversion techniques
19MS605.4	.Understand the various approaches for nanomaterials synthesis

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS605.1	2	2	2	1								
19MS605.2	3	2	2		2							
19MS605.3	3	2			2							
19MS605.4	2	3	3	2								

## **19MS611 MATERIALS CHARACTERIZATION TECHNIQUES**

**4-0-0-4**

Atomic and Molecular Spectroscopy: Atomic Absorption, Fluorescence and Emission Spectroscopy, UV-Visible Spectroscopy, Infrared Spectroscopy, Raman Spectroscopy, Energy Dispersive X-ray Spectroscopy, X-ray Photoelectron Spectroscopy, Nuclear Magnetic Resonance Spectroscopy, Mass Spectrometry;

Imaging Microscopies and Image Analysis: Optical Microscopy, Scanning Electron Microscopy, Scanning Probe Microscopy, Image Analysis;

X-ray and Electron Diffraction: Properties of X-Rays, Review of Crystal Systems and Miller Indices, Stereographic Projections, The Reciprocal Lattice, Laue Equations, Diffraction Methods, Scattered Intensities, Phase Identification, Small angle scattering;

Thermal and Thermomechanical Techniques: Differential Scanning Calorimetry and Differential Thermal Analysis, Thermogravimetric Analysis, Dynamic Mechanical Analysis and Thermomechanical Analysis.

#### TEXTBOOKS/REFERENCES:

1. D. A. Skoog, F. J. Holler and S. R. Crouch, "*Principles of Instrumental Analysis*", Sixth Edition, Cengage Learning, New Delhi, 2007.
2. B. D. Cullity and S. R. Stock, "*Elements of X-ray Diffraction*", Third Edition, Prentice Hall Inc., New Jersey, 2001.
3. K.P. Menard, "*Dynamic Mechanical Analysis; A Practical Introduction*", CRC Press, Boca Raton, 1999.
4. S. Zhang, L. Li and A. Kumar, "*Materials Characterization Techniques*", CRC Press, Boca Raton, 2008.
5. Y. Leng, "*Materials Characterization: Introduction to Microscopic and Spectroscopic Methods*", Second Edition, Wiley-VCH, 2013.

CO Code	Course outcome statement
19MS611.1	Understand the fundamental principles behind the individual characterization methods which are included in the curriculum.
19MS611.2	Analyze, interpret and present observations from the different characterization methods.
19MS611.3	Assess which methods of characterization are appropriate for different material / requirement/ condition/ problems.
19MS611.4	Able to evaluate the uncertainty of observations and results from the different characterization methods.

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS611.1	2	3	1	1	2							
19MS611.2	2	3	3	2	2							
19MS611.3	2	3	3	2	2							
19MS611.4	2	2	3	3	3							

Review of Crystal Structure and Defects; Mechanical Properties of Metals and Alloys: Tensile, Impact, Hardness, Creep; Elastic Deformation: Characteristics of Elastic Deformation, Atomic Mechanisms of Elastic Deformation; Inelastic Deformation: Strain–Time Curves; Plastic Deformation: Mechanism of Plastic Deformation, Slip and Twinning; Strengthening Mechanisms: Work Hardening, Grain Boundary Hardening, Dispersion Hardening; Creep: Primary, Secondary and Tertiary Creep; Fracture: Ideal Fracture Stress, Brittle Fracture, Griffith’s Theory, Cup and Conetype Fracture, Schmidt’s Law, Critical Resolved Shear Stress; Fatigue: S-N curves, Endurance Limit; Materials Damage: Wear, Corrosion, Failure

Phase Diagrams of Non-Ferrous Systems: Brass, Bronze, Aluminum, Magnesium, Nickel, Lead, Tin, Titanium, Zinc Alloys; Steel: Heat Treatment, Alloy Steels: Influence of Alloying Elements on Iron-Iron Carbide Phase Diagram, Effects on Properties of Steel, Stainless Steels: Austenitic, Martensitic, Ferritic, Heat-Resistant Steels, Maraging Steels, Tool Steels

**TEXTBOOKS/REFERENCES:**

1. W.D. Callister, “*Materials Science and Engineering*”, Sixth Edition, John Wiley & Sons, 2003.
2. S. H. Avner, “*Introduction to Physical Metallurgy*”, Second Edition McGraw Hill, 1997.
3. R. E. Reed-Hill, “*Physical Metallurgy Principles*”, Affiliated East-West Press, 2008.
4. G. E. Dieter, “*Mechanical Metallurgy*”, McGraw Hill Education, 2017.
5. V. Raghavan, “*Materials Science and Engineering: A First Course*”, Fifth Edition, Prentice Hall India, 2004.

CO Code	Course outcome statement
19MS612.1	Recall the structure of solids and the various crystal imperfections.
19MS612.2	Understand the types of deformations in solids and the failure patterns.
19MS612.3	Suggest testing methodologies for the characterization of different categories of materials
19MS612.4	Interpret phase diagrams of alloys with special reference to Iron-Carbon and nonferrous systems
19MS612.5	Understand the concept of heat treatment of steels & strengthening mechanisms

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
---------	-----	-----	-----	-----	-----	-----	-----	-----	-----	-------	-------	-------

19MS612.1	2	2	2	1								
19MS612.2	3	2	2		2							
19MS612.3	3	2			2							
19MS612.4	2	3	3	2								

### 19MS613

### ADVANCED MATERIALS

4-0-0-4

Nanomaterials Fundamentals: Atomic Structure, molecules and phase, 0-D, 1-D, 2-D and 3-D nanomaterials, nanostructured metals, MO<sub>x</sub>, MS<sub>x</sub>, and nanocarbon; structure-property relationships – optical, catalytic, mechanical, thermal, electrical properties; MEMS and NEMS nanoscale Optoelectronics

Polymers: Types, Commodity Plastics: PE, PP, PVC, PS; Engineering Plastics: PA, Fluoropolymers, Polyesters; Thermosets – Phenolics and Epoxy Resins; Rubbers: Natural and Synthetic, Additives; High-Performance Polymers: PEEK; Structure-Property Relationships: Chemical Properties, Solubility, Mechanical Properties, Calorimetric Properties, Electrical Properties, Optical Properties, Acoustic Properties, Processability; Smart Materials: Shape Memory Alloys, Super Alloys, High Entropy Alloys, Magnetorheological and Electrorheological Fluids, Gels

#### TEXTBOOKS/REFERENCES:

1. M. A. Ratner and D. Ratner, “*Nanotechnology: A Gentle Introduction to the Next Big Idea*”, Prentice Hall, 2002.
2. M. Wilson, K. Kannangara, G. Smith, M. Simmons and B. Raguse, “*Nanotechnology: Basic Science and Emerging Technologies*”, Chapman and Hall, 2002.
3. A. Nouailhat, “*An Introduction to Nanosciences and Nanotechnology*”, Wiley-ISTE, 2008.
4. J. A. Brydson, “*Plastics Materials*”, Butterworth-Heinemann, Seventh Edition, Oxford, 1999.
5. M. Morton, “*Rubber Technology*”, Third Edition, Kluwer Academic Publishers, Dordrecht, Netherlands, 1999.

CO Code	Course outcome statement
19MS613.1	Outline the structure, properties and applications of nanomaterials
19MS613.2	Outline the structure, properties, processing and applications of common thermoplastics, thermosets and elastomers.
19MS613.3	Summarize the properties and applications of some smart materials and systems

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS613.1	3	2	2	1	1				1	1		1
19MS613.2	3	2	2	1	1				1	1		1
19MS613.3	3	2	2	1	1				1	1		1

## 19MS614

## MATERIALS DESIGN

3-0-0-3

Structure-Property-Function Relationships in Materials, Process-Property Interaction, Material Property Charts, Design through Materials Synthesis and Modification, Materials and Process Information for Design; Translation, Screening and Ranking of Materials, Manipulating Properties - Density, Mechanical, Thermal, Electrical, Magnetic, Optical, Reactivity, and Catalytic Properties

Selected Case Studies: Ball Milling, Sintering, Layered Compounds, Chemical Vapor Deposition of Solids, Crystal Growth, Hydrothermal Synthesis, Sol-Gel Process, Polymer Synthesis, Gas-Phase Pyrolysis for Liquids, Catalytic Control of Fischer-Tropsch Process for Engine-Grade Fuels, Nanomaterials: Nanoparticles, Soft Templating, Self-Assembled Monolayers, Hard Templating - Nanocasting, Nanowires using Templated Deposition, Chemical Synthesis of Graphene, Graphene Functionalization for Applications, Biomaterials: Designing Bone Scaffolds, Contact Lenses

### TEXTBOOKS/REFERENCES:

1. M. Ashby, H. Shercliff and D. Cebon, "*Materials: Engineering, Science, Processing and Design*", Second Edition, Butterworth-Heinemann, 2010
2. U. Schubert and N. Hüsing, "*Synthesis of Inorganic Materials*", Third Edition, Wiley-VCH, 2012
3. Selected recent papers published in reputed international journals discussing materials design - for case studies

CO Code	Course outcome statement
19MS614.1	Understand the material manufacturing process tree and material property charts
19MS614.2	Understand the materials design and materials selection process
19MS614.3	Able to recall the material properties, such as mechanical, electrical, thermal, magnetic and electrochemical properties.

19MS614.4	Able to manipulate the material properties to fit in specific applications
-----------	--

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS614.1	3	2			2				1			2
19MS614.2	3	2	1	2	1				1			2
19MS614.3	3	2										2
19MS614.4	2	3	3	3	2							1

### **19MS615 MATERIALS SYNTHESIS AND CHARACTERIZATION LAB – I 0-0-2-1**

The lab will comprise hands-on materials synthesis experiments along with their characterization with focus on interpretation.

Synthesis of materials: bulk polymerization, hydrothermal synthesis, electrodeposition of copper, Hummers method for graphene oxide, ball milling of nanostructured metal powders and sintering

Characterization of materials: viscosity and molecular weight, UV-visible spectroscopy, IR spectroscopy, thermogravimetric analysis, differential scanning calorimetry, optical microscopy and metallography, dynamic light scattering

CO Code	Course outcome statement
19MS615.1	Choose appropriate methods, understand underlying principles, perform experiments, analyse obtained results and interpret outcomes for polymerization, polymerization mechanisms, determination of structure (bonds, functional groups), determination of properties (molecular weight, viscosity, glass transition, viscoelastic)
19MS615.2	Understand principles of hydrothermal synthesis, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained nanomaterials, their structure (bonds, functional groups, crystallinity and crystal structure, morphology and composition) and properties (light absorption, band gap)

19MS615.3	Understand principles of electrodeposition, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained thin films, their structure (crystallinity, crystal structure, film thickness, morphology and composition) and properties
19MS615.4	Understand principles of milling and sintering of metal powders to form compacted metal structures, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained materials, their structure (size, crystallinity, crystal structure, film thickness, morphology and composition) and properties (mechanical)
19MS615.5	Understand complex materials synthesis processes with multiple steps such as Hummers method, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained graphene oxides, their structures (functional groups, crystallinity, crystal structure, number of layers, morphology and composition) and properties (optical)

CO Code	PO 1	PO 2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS615.1	3	3	3	3	3		1	1	3	3	2	3
19MS615.2	3	3	3	3	3		1	1	3	3	2	3
19MS615.3	3	3	3	3	3		1	1	3	3	2	3
19MS615.4	3	3	3	3	3		1	1	3	3	2	3
19MS615.5	3	3	3	3	3		1	1	3	3	2	3

### **19MS616 MATERIALS SYNTHESIS AND CHARACTERIZATION LAB – II 0-0-2-1**

The lab will comprise hands-on materials synthesis experiments along with their characterization with focus on interpretation.

Synthesis of materials: Sol-gel synthesis, solid-state synthesis, spray pyrolysis, self-assembly of monolayers, chemical and ultrasonication-assisted reduction of graphene oxide, electrodeposition of alloys, injection moulding

Characterization of materials: X-ray diffraction, gas chromatography, mass spectrometry, cyclic voltammetry, contact angle and surface tension, scanning electron microscopy, energy dispersive Xray spectroscopy

CO Code	Course outcome statement
19MS616.1	Understand the principles behind synthesis of nanomaterials such as sol-gel and solid-state synthesis, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained materials, their structure (crystallinity, crystal structure, film thickness, morphology and composition) and properties
19MS616.2	Understand the principles behind thin film synthesis techniques, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained materials, their structure and properties
19MS616.3	Understand complex materials synthesis processes with multiple steps such as reduction of graphene oxide, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained materials, their structure and properties
19MS616.4	Understand component manufacturing processes such as injection moulding, perform experiments, analyse obtained results and interpret outcomes (effects of synthesis conditions) of obtained components, their structure and properties

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
19MS616.1	3	3	3	3	3		1	1	3	3	2	3
19MS616.2	3	3	3	3	3		1	1	3	3	2	3
19MS616.3	3	3	3	3	3		1	1	3	3	2	3
19MS616.4	3	3	3	3	3		1	1	3	3	2	3

### **19MS617 MATERIALS PERFORMANCE ANALYSIS LAB**

**0-0-2-1**

Hardness Test, Impact Test, Tensile/Compression Test, Three-Point Bending Analysis, Uv-visible Spectroscopy - Transparency of a Thin Film, Photocatalytic Degradation of a Volatile Organic Compound, Electrical Conductivity - Ac and Dc, Magnetoresistance, Charge-Discharge of Batteries, Charge-Discharge Behavior of Capacitor, Hall Effect Measurement, I-V Characteristics of a Solar Cell, Energy Storage in a Phase Change Material

CO Code	Course outcome statement
19MS617.1	Ability to conduct experiments to validate thermal and electrical behaviour of materials
19MS617.2	To evaluate the mechanical behaviour of materials under different loading conditions.
19MS617.3	Suggest materials testing techniques based upon desired results, perform analysis on data, and present test results in a written format

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS617.1	3	2	2	2					2			1
19MS617.2	3	2		1	2				2			1
19MS617.3	2	2	2		2				1			2

## ELECTIVES

**19MS701**

**POLYMER PROCESSING**

**3-0-0-3**

Physical Basis of Polymer Processing- Mixing- Types of mixing process. Extrusion-Features of a Single Screw Extruder, Analysis of Flow, Aspects of Screw Design, Operating Point. Twin Screw Extrusion-Processes - Pipe, Profile, Blown Film, Wire and Cable coating, Fibre, Film and sheet extrusion, Co extrusion-Melt Fracture-Sharkskin-Die swell. Injection Moulding-Principles-Moulding Cycle-Reciprocating Screw Injection Moulding Machine-Types of Clamping Units-PVT diagram Aspects of Product Quality-Hot Runner Moulding-Gas Assisted Injection Moulding. Blow Moulding-Principles-Injection Blow Moulding-Extrusion Blow Moulding-Stretch Blow Moulding Troubleshooting-Thermoforming-Vacuum Forming-Pressure Forming-Material Stress and Orientation-Applications in Packaging. Compression and Transfer Moulding-Thermosetting Compounds-Flash, Semi Positive, Positive Type Moulds-Types of Moulding Machines-Transfer Moulding-Troubleshooting-Comparison. Fibre Reinforced Plastics-Materials-Lay-up processes-SMC, DMC-Resin Transfer Moulding- Pultrusion, Bag Moulding Processes-Filament Winding Process Variants-Newer developments using thermosets. Polymers in Rubbery State-Calendering Process-Types of Calendars, Roll Deflection, Roll Cambering-Rotational Moulding-Types of Machines, Moulds, Materials. Joining and Machining of Plastics-Welding of Plastics-Ultrasonic, Induction, Hotplate, High Frequency-Solvent Cementing-Adhesive Bonding.

Introduction – Rheological parameters stress, strain and rate of deformation - Newtonian and Non Newtonian fluids – time dependent fluids – isothermal viscous flow in tubes – Entrance and exit effects - elastic effects in polymer melt flow - die- swell and melt fracture – Weissenberg effect - Extensional Viscosity. Measurement of rheological properties – capillary rheometers – melt flow indexer – cone and plate viscometer – torque rheometers – Mooney viscometer.– Applications of rheology to polymer processing [injection moulding, extrusion, blow moulding, two roll mill - calender] . Mechanical models – Maxwell element – Voigt Kelvin element – Boltzmann and time temperature superposition principles – WLF equation.

#### TEXTBOOKS/REFERENCES:

1. D. H. Morton – Jones, “Polymer Processing”, Chapman and Hall, New York, 1996.
2. Michael L Berins (ed), “Plastics Engineering Handbook Society of Plastics Industry”, Kluwer Academic Publishers, 2000
3. B. R. Gupta, “Applied Rheology in Polymer Processing”, Asian Books Pvt Ltd, New Delhi, 2005
4. R. J. Crawford, “Plastics Engineering”, Butterworth-Heinemann, Oxford, 1998
5. D.V. Rosato and Rosato, “Injection Moulding Handbook Complete Molding Operatio, Technology, Performance and Economics”, CBS Publishers New Delhi, 1987.
6. Chris Rauwendaal, “Polymer Extrusion”, Hanser, 2001.
7. A. Brydson, “Flow Properties of Polymer Melts”, Illife Books, London, 1978.
8. John M. Dealy and Kurt F. Wissburn, “Melt Rheology and its Role in Plastics Processing”, Chapman, London, 1995.

CO Code	Course outcome statement
19MS701.1	Gain an overview of different type of polymer processing techniques : Injection, extrusion, blow, thermoforming, compression and transfer moulding, composites processing
19MS701.2	Understand the parameters and troubleshooting techniques specific to various polymer processing operations
19MS701.3	Understand the rheological properties of the polymers and their influence in polymer processing

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
19MS701.1	3		1								2	1
19MS701.2	3	2	3									2
19MS701.3	3	2	2		2							2

Fundamentals of Electrochemistry: Arrhenius theory of dissociation, Solvation, Mobility, Transport Number; Ionics: Guoy-Chapman and Debye-Huckel theories of ion-ion interaction; Electrified Interface: Structure of electrode-electrolyte interface – Non-Faradaic processes, Thermodynamic activity, Electrochemical potential and Nernst Equation; Mass Transfer in Electrolytes – Convection, Diffusion, and Migration; Electrode Kinetics – Butler-Volmer Equation, Tafel Equation, Polarization of Electrodes – Activation and Concentration polarization, Reaction Mechanisms in Electrochemistry – Rate Laws; Electroanalytical Techniques: Conductometric and Potentiometric Titrations, Potential Step Methods – Chronoamperometry, Potential Sweep Methods – Linear Sweep Voltammetry and Cyclic Voltammetry: Reversible, Quasireversible, and Irreversible Systems; Pulse Voltammetry – Normal Pulse, Differential Pulse, and Square Wave Voltammetry; Electrochemical Impedance Analysis; Selected Applications such as Electrodeposition of Alloys, Corrosion, Batteries, Fuel Cells, and Electrochemical Sensors

**TEXTBOOK/REFERENCE:**

1. J. O'M. Bockris and A. K. N. Reddy, "*Modern Electrochemistry*" Volumes 1, 2A, and 2B, Second Edition, Kluwer Academic Publishers, NY, 2000
2. A. J. Bard and L. R. Faulkner, "*Electrochemical Methods: Fundamentals and Applications*", Second Edition, John Wiley and Sons, NY, 2001
3. V. S. Bagotsky, "*Fundamentals of Electrochemistry*", Second Edition, Wiley-Interscience, 2006

CO Code	Course outcome statement
19MS702.1	Understand how ions behave in solution by way of ion-solvent and ion-ion interactions. Understand and explain the theories that capture this behaviour and analyse how they affect ion mobility and transport number in an electrolyte.
19MS702.2	Understand and describe the structure of an electrified double layer. Analyse the non-Faradaic processes that take place in electrochemical systems. Develop and
	apply thermodynamic principles for electrochemical systems.
19MS702.3	Understand how mass transport occurs in electrochemical systems. Develop and apply relations to interpret the behaviour of electrochemical systems under diffusion-controlled conditions.
19MS702.4	Understand how an electrochemical reaction takes place at an electrode-electrolyte interface. Derive and apply the relevant equations for electrode kinetics in different electrochemical systems. Understand polarization and how the different polarizations affect the Faradaic response of an electrochemical system.

19MS702.5	Understand how different electroanalytical techniques may be constructed to analyse an electrochemical system. Develop and apply the basic principles and equations of techniques such as chronoampero/coulometry, linear/cyclic voltammetry, pulse voltammetry and electrochemical impedance spectroscopy to analyse electrochemical processes.
19MS702.6	Understand the principles and forms of corrosion. Analyse how various factors influence the rate of corrosion. Apply electroanalytical techniques to understand corrosion behaviour. Describe the different methods to control corrosion and evaluate their applicability under different conditions.

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS702.1	3	2	2	1					2	1		1
19MS702.2	3	2	2	1					2	1		1
19MS702.3	3	3	3	3					2	1		1
19MS702.4	3	3	3	3					2	1		1
19MS702.5	3	3	3	3					2	1		1
19MS702.6	3	3	3	3					2	1		1

### 19MS703

### CATALYTIC CHEMISTRY

3-0-0-3

Catalysis – introduction, Catalyst and catalysis, positive and negative catalysis, Type of catalysis, Characteristics of catalytic reactions, promoters, Catalytic poisoning, Catalysis in gas phase – examples, Catalysis in solution phase – Homogeneous catalysis – acid base catalysis, oxidation reactions, heterogeneous catalysis – introduction, organometallic catalysis, metallocenes, Ziegler Natta catalyst, phase transfer catalysts and various industrially employed reactions

Enzyme catalysis –introduction, classification, mechanism of enzyme catalysis, characteristics of enzyme catalysis, metalloenzymes, solid support, application of catalysis in industries.

Catalysis by zeolites – introduction, classifications, synthesis, examples of various reactions and functional modification on zeolite surface.

#### TEXTBOOK/REFERENCES:

1. Catalytic Chemistry, Bruce C Gates, John Wiley and sons USA (1992)
2. Concise Coordination Chemistry, Gopalan and Rajalingam
3. Physical Chemistry for Engineering Students, Puri, Sharma and Pathania
4. Principles of Chemical Kinetics, James E house, Academic press (2007)

5. Catalysis, Principles and Applications, Viswanathan, Sivashankar and Ramaswamy, CRC press (2006).

CO Code	Course outcome statement
19MS703.1	Understand the fundamentals, types and characteristics of catalysis
19MS703.2	Able to understand the catalytic reactions in gas phase and solution phase
19MS703.3	Able to understand homogeneous catalysis and heterogeneous catalysis
19MS703.4	Able to understand the enzyme catalysis and catalysis by zeolites.

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS703.1	3	3	2	1	2							1
19MS703.2	3	2	2	1	2							1
19MS703.3	3	2	2	1	2							1
19MS703.4	3	1	2	1	2							1

#### 19MS704

#### CARBON NANOMATERIALS

3-0-0-3

Graphene: Synthesis, Properties, and Applications; Fullerene C60 Architectures in Materials Science; Graphite Whiskers, Cones, and Polyhedral Crystals; Epitaxial Graphene and Carbon Nanotubes on Silicon Carbide; Cooperative Interaction - Crystallization, and Properties of Polymer–Carbon Nanotube Nanocomposites; Carbon Nanotube Biosensors; Carbon Nanostructures in Biomedical Applications, Field Emission from Carbon Nanotubes; Nanocrystalline Diamond; Carbon Onions; Carbide-Derived Carbons; Templated and Ordered Mesoporous Carbons; Oxidation and Purification of Carbon Nanostructures; Hydrothermal Synthesis of Nano-Carbons; Carbon Nanomaterials for Water Desalination by Capacitive Deionization; Carbon Nanotubes for Photoinduced Energy Conversion Applications;

#### TEXTBOOKS/REFERENCES:

1. Yury Gogotsi, Volker Presser, “Carbon Nanomaterials”, 2<sup>nd</sup> ed., CRC Press, 2013
2. Francis and Karl M. Kadish, “Handbook of Carbon Nanomaterials”, Vol.1&2, World Scientific, 2011

CO Code	Course outcome statement
19MS704.1	Describe the methods of synthesizing and modifying carbon nanomaterials including graphene, fullerenes, CNTs, Graphite whiskers, cones, and polyhedral crystals.
19MS704.2	Explain the methods of characterizing carbon nanomaterials.
19MS704.3	Apply carbon nanomaterials in the fields of biosensors, biomedicine, water desalination, and photo-induced energy conversion.

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
19MS704.1	2			3	1				1	1		1
19MS704.2	2	2		2	1				1	1		1
19MS704.3			3			2	2		1	1		1

### **19MS705 INTERFACIAL SCIENCE & ENGINEERING 3-0-0-3**

Introduction to Surfaces, Interfaces, and Colloids; Surface and Interface – Molecular Origin, the work of cohesion and adhesion, Surfactants structure, types Interaction forces and potential, chemical and physical interaction, classification of physical forces. Van der Waals force, interaction between surface and particles - Electrostatic forces and electric double layer; DLVO theory, Hamaker constant, Boltzmann distribution, Debye length, specific ion adsorption, ion adsorption, Stern layer, Electrostatic, steric and electrosteric stabilization, zeta potential, surface tension, wetting and spreading, Young's equation, contact angle - Solid surfaces - surface mobility, characteristics, formation; Adsorption, energy consideration of physical adsorption vs. chemisorptions, Gibbs surface excess, Gibbs adsorption equation, Langmuir isotherm, BET isotherm, adsorption at solid-liquid interfaces - Stability of colloids – Emulsions, formation and stability, HLB number, PIT (phase inversion temperature) Foams, Aerosols, Microemulsions, Vesicles, Micelles and Membranes - Applications of various colloidal systems

#### **TEXTBOOKS/REFERENCES:**

1. D. Myers, "Surfaces, Interfaces, and Colloids: Principles and Applications", 2<sup>nd</sup> Edition, WileyVCH, 1999.

2. T. Cosgrove, "Colloid Science: Principles, Methods and Applications", 2<sup>nd</sup> Edition, WileyBlackwell, 2010.
3. P.C. Hiemenz and R. Rajagopalan (Editors), "Principles of Colloid and Surface Chemistry", 3<sup>rd</sup> Edition, Academic Press, New York, 1997.

CO Code	Course outcome statement
19MS705.1	Understand the fundamental theories associated with the surface and interface properties
19MS705.2	Study the surface and interfacial phenomena of thin film coatings and colloids
19MS705.3	Analyze the role of surface and interface properties in the processings of different industrial products, intermediates and raw materials
19MS705.4	Design of new product formulations with superior surface and interface properties

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO10	PO11	PO12
19MS705.1	3	2	2	1	1	1	1					
19MS705.2	2	2	2	2	2	1						
19MS705.3	2	2	3	3	3							
19MS705.4	2	2	3	3	3	1						

## 19MS706

## WASTE TO ENERGY

## 3-0-0-3

Waste – energy content, waste classification, waste composition, and waste segregation; Introduction to gasification, pyrolysis and combustion technology(s); Pyrolysis of waste to liquid fuels – Thermal, catalytic / thermal, catalyst and reactor choice for pyrolysis; Gasification to Liquid fuels via synthesis gas route – Petrol and Diesel production, Processes for waste to value-added chemicals via synthesis gas– Hydrogen production, methanol production, ethanol production – Design and catalyst choice for various technologies; Gasification to Electricity – A Case study; Biomass – Classification and Composition; Biomass pyrolysis and gasification to engine grade fuels – catalyst and equipment design.

### TEXTBOOKS/REFERENCES:

1. Gary C. Young, *Municipal Solid Waste Conversion Processes*, John Wiley & Sons Inc., 2010

2. Marc J. Rogoff and Francois Screve, *Waste to Energy: Technologies and Project Implementation*, 2<sup>nd</sup> Edition, Elsevier Inc., 2011.
3. Avraam Karagiannidis, *Waste to Energy*, Springer-Verlag Limited., 2012

CO Code	Course outcome statement
19MS706.1	Classify waste based on energy content, phase and composition.
19MS706.2	Establish a relationship between composition and energy content of the waste.
19MS706.3	Analyze effect of feed variation and process parameters on waste to energy conversion processes and optimize the same for required output.
19MS706.4	Evaluate the kinetics of waste to energy process / technologies - Combustion, gasification and pyrolysis

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS706.1	2	2	1	1	1	1	3	-	1	2		
19MS706.2	3	3	3	3	2	2	3	-	2	2		2
19MS706.3	3	3	3	3	3	3	3	-	2	2		
19MS706.4	2	2	3	3	3	2	3	-	2	1		3

## 19MS707

## SOLAR ENERGY

## 3-0-0-3

Solar energy: Solar radiation, its measurements and analysis. Solar angles, day length, angle of incidence on tilted surface, Sun path diagrams, Shadow determination. Extraterrestrial characteristics, Effect of earth atmosphere, measurement & estimation on horizontal and tilted surfaces. Solar cell physics: p-n junction, homo and hetero junctions, Metal-semiconductor interface, Dark and illumination characteristics, Figure of merits of solar cell, Efficiency limits, Variation of efficiency with band-gap and temperature, efficiency measurements, high efficiency cells, Tandem structure. Solar cell fabrication technology: Preparation of metallurgical, Electronic and Solar grade Silicon, Production of Single Crystal 'Si', Chocharl'ski (CZ) and Float Zone (FZ) method for preparation of silicon, procedure of masking, photolithography and etching, Design of a complete silicon, GaAs, InP solar cell. High efficiency III-V, II-VI multijunction solar cell, a-Si-H based solar cells, Quantum well

solar cell, Thermophotovoltaics. Nanosolar cells. Solar photovoltaic system design: Solar cell arrays, system analysis and performance prediction, shadow analysis, reliability, solar cell array design concepts, PV system design, Design process and optimization, Detailed array design, storage autonomy, Voltage regulation, maximum tracking, Power electronic converters for interfacing with load and grid, use of computers in array design, Quick sizing method, Array protection and troubleshooting; Solar Photovoltaic applications – detailed design and economics; Solar Thermal systems: Solar thermal collectors, flat plate collectors, concentrating collectors, solar heating of buildings, solar still, solar water heaters, solar driers; conversion of heat energy in to mechanical energy, solar thermal power generation systems.

#### TEXTBOOKS/REFERENCES:

1. J. W. Twidell and A.D. Weir, “*Renewable Energy Resources*”, Second Edition, Taylor & Francis, New York, 2005.
2. H.P. Garg and J. Prakash, “*Solar Energy: Fundamentals & Applications*”, Tata McGraw Hill, New Delhi, 1997.
3. S.P. Sukhatme and J.K. Nayak, “*Solar Energy: Principles of Thermal Collection and Storage*”, Third Edition, McGraw Hill, New York, 2009.
4. J.F. Kreider and F. Kreith, “*Solar Energy Handbook*”, McGraw Hill, New York, 1981.
5. D.Y. Goswami, F. Kreith and J.F. Kreider, “*Principles of Solar Engineering*”, Second Edition, CRC Press, Boca Raton, 2000.

CO Code	Course outcome statement
19MS707.1	Calculate the solar radiation at a given location, time and tilt.
19MS707.2	Compare the methods of synthesis and characterization of different solar cells based on Si, GaAs, InP, III-V, II-VI multijunctions, a-Si-H, quantum wells.
19MS707.3	Design simple photovoltaic systems
19MS707.4	Outline the main solar thermal devices and systems

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS707.1	3				2				1	1		1
19MS707.2	3	2		1					1	1		1
19MS707.3			3		2	1	2		1	1	2	1

19MS707.4			2			1	2		1	1		1
-----------	--	--	---	--	--	---	---	--	---	---	--	---

**19MS708**

**ENERGY STORAGE TECHNOLOGIES**

**3-0-0-3**

Introduction to energy storage, need for energy storage and different modes of energy storage. Electrochemical Energy storage - Supercapacitors, Materials for Supercapacitors, Batteries, Lead-Acid Batteries, Nickel-Metal Hydride batteries, Lithium-Ion Batteries, Thin-film Batteries, Metal Air Batteries, Energy Storage for Fuel Cells; Hydrogen storage- Hydrogen Economy, Different modes of hydrogen storage, compressed gas storage, liquid hydrogen storage, metal hydrides, Advanced Materials for Solid-State hydrogen storage; Role of carbon materials in energy conversion and storage - carbon nanotubes, graphene; Other Types of Energy Storage – Flywheels, Superconducting Magnetic Energy Storage (SMES), Pumped Storage Hydroelectricity (PHS), Compressed Air Energy Storage (CAES); Electrolysis of water and Methanation; Electrical energy storage; Thermal Storage; Hydraulic Hydro Energy Storage (HHS); Energy Storage technologies for wind power integration

**TEXTBOOKS/REFERENCES:**

1. Tetsuya Osaka, Madhav Datta , “*Energy Storage Systems in Electronics*”, 1<sup>st</sup> ed., CRC Press , 2000.
2. David Michael Rowe, “*Thermoelectrics Handbook: Macro to Nano*”, CRC Press, 2006.

CO Code	Course outcome statement
19MS708.1	Able to understand the concept of kinetic and thermodynamic aspects of electrochemical reactions and able to correlate the electrode kinetics with battery operation.
19MS708.2	Able to understand the different battery technologies and differentiate with respect to performance and operating conditions
19MS708.3	Able to understand the concept of solid-state hydrogen storage and supercapacitor materials and their advantages and disadvantages.
19MS708.4	Able to understand other storage technologies, such as mechanical and thermal energy storage.

CO Code	PO 1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS708.1	3	2		3								1

19MS708.2	3	2	2	2	2	1	1					1
19MS708.3	3	2	2	2	2	1	1					1
19MS708.4	3	2	2	2	2	1	1					1

## 19MS709

## MOLECULAR SIMULATION

1-0-2-3

Definitions, Scope; Approaches for Molecular Simulation; Statistics – Estimating Macroscopic Properties from Molecular Simulations; Quantum Mechanics, Symmetry and Group Theory – Representing Molecules and Molecular Interactions; Molecular Orbital Theory; Hartree-Fock Approach; Density Functional Theory; Molecular Mechanics – Energy and Forces for Molecular Interactions; Constraints; Periodic Boundaries and Neighbor Lists; Introduction to Monte Carlo (MC) Simulations and Molecular Dynamics (MD); Minimization of functions – Advanced Energy Minimization Techniques

Introduction to Unix; Software for Molecular Modeling (any two): GROMACS, ABINIT, ADUN, CP2K, CHARMM, DALTON, NAMD, LAMMPS, SPARTAN, TINKER; Programming Exercises (any five): Evaluation of Pi (MC), Pair-correlation functions, Integration using MC, MD of a simple fluid, MD of an excluded-volume polymer chain, 3D Visualization of Molecules, Model Building, Energy Minimization, Dynamics, Surface Properties, Thermodynamic Properties, Electronic Structure Calculations, Electronic Transport Properties; Case Studies

### TEXTBOOKS/REFERENCES:

1. K. I. Ramachandran, D. Gopakumar and K. Namboori, “*Computational Chemistry and Molecular Modeling: Principles and Applications*”, Springer, 2008.
2. T. Schlick, “*Molecular Modeling and Simulation: An Interdisciplinary Guide*”, Springer, 2002.
3. D. Frenkel and B. Smit, “*Understanding Molecular Simulations: From Algorithms to Applications*”, Second Edition, Academic Press, 2002.
4. M. P. Allen and D. J. Tildesley, *Computer Simulation of Liquids*, Clarendon Press, 1987.
5. Journal articles on molecular simulation of molecules of interest.

CO Code	Course outcome statement
19MS709.1	Classify molecular simulation approaches, understand their scope and applicability and determine the suitability of simulation approaches for materials engineering problems.
19MS709.2	Understand the statistics in estimating macroscopic properties from molecular simulations and employ principles of thermodynamics and transport processes for the same.

19MS709.3	Understand the quantum mechanical model of atoms, molecules and their interactions. Understand the principles and algorithms of quantum mechanical simulations such as Hartree-Fock, DFT, Ab Initio and Semi-Empirical simulations.
19MS709.4	Apply models of molecular interactions in molecular dynamics and Monte Carlo simulations, understand different algorithms in these simulations and minimization of energy.
19MS709.5	Gain hands-on skills in at least two simulation techniques, analyse case studies and simulate model cases.

CO Code	PO1	PO2	PO3	PO4	PO5	PO6	PO7	PO8	PO9	PO 10	PO 11	PO 12
19MS709.1	3	3	3	3	3				2	2		2
19MS709.2	3	3	3	3	3				2	2		2
19MS709.3	3	3	3	3	3				2	2		2
19MS709.4	3	3	3	3	3				2	2		2
19MS709.5	3	3	3	3	3				2	2		2

## 19MS710

## DESIGN FOR SUSTAINABLE DEVELOPMENT

3-0-0-3

Introduction: Sustainability, Need for Design, interdisciplinary holistic approach. Fundamental concepts: Physics, Thermodynamics, Flow, Stoichiometry, biological processes.

Philosophy of Sustainability: Fundamental causes of unsustainability, justice and sustainability ethics, societal and personal goals. Principles of Sustainable Design: The design process, cyclical design, goal-based design, systems thinking, LCA, EIA, resource management, socio-economic considerations. Case studies: Building, Water, Agriculture, Energy, Transportation, Industrial symbiosis.

### TEXTBOOKS/REFERENCES:

1. Daniel Vallero and Chris Brasier, *Sustainable Design: The Science of Sustainability and Green Engineering* John Wiley & Sons, Inc., Hoboken, New Jersey, 2008. ISBN 978-0-470-13062-9.
2. W. McDonough and M. Braungart, *Cradle to Cradle: Remaking the Way We Make Things*, North Point Press, New York, 2002.
3. J. M. Benyus, *Biomimicry*, William Morrow, New York, 1997.
4. B. B. Marriott, *Environmental Impact Assessment: A Practical Guide*, McGraw-Hill, New York, 1997.

<b>CO Code</b>	<b>Course outcome statement</b>
19MS710.1	Identify the need for a holistic design approach to achieving sustainability
19MS710.2	Identify the ethical roots of unsustainability and identify ethics as a prerequisite for sustainable design
19MS710.3	Design cyclical and sustainable systems meeting the triple bottom line

<b>CO Code</b>	<b>PO1</b>	<b>PO2</b>	<b>PO3</b>	<b>PO4</b>	<b>PO5</b>	<b>PO6</b>	<b>PO7</b>	<b>PO8</b>	<b>PO9</b>	<b>PO 10</b>	<b>PO 11</b>	<b>PO 12</b>
19MS710.1	3	2				2	2	2	1	1		1
19MS710.2						3	3	3	1	1		2
19MS710.3	2		3			3	3	2	1	1		2