M.Tech. in Materials Engineering

(Specialization in Functional Materials)

Program structure with courses

Cat.	Course Number, Course Title		L-T-P	Credits		Cat.	Course Number, Course Title		L-T-P	Credits
I Semester						**II Semester**				
C	MTL7XX0	Thermodynamics of Materials	2-0-2	3		C	MTL7XX0	Functional Materials	3-0-0	3
C	MTL7XX0	Characterization of Materials	2-0-2	3		E	MTL7XX0	*Elective*	3-0-0	3
C	MTL7XX0	Symmetry, Structure and Tensor Properties	3-0-0	3		E	MTL7XX0	*Elective*	3-0-0	3
E	MTL7XX0	Elective	3-0-0	3		E	MTL7XX0	*Elective*	3-0-0	3
NG1	LAN7XX0	*Technical Communication*	1-0-0	S/U		NG2	OAL7XX0	*Innovation and IP Management*	1-0-0	S/U
			Total	**12**					*Total*	**12**
T	MTS 7xx0	*Summer Thesis*								**8**
III Semester						**IV Semester**				
T	MTT7XX0	Thesis		16		T	MTT7XX0	Thesis		16
			Total	**16**					*Total*	**16**

S.No.	Category	Course Category Title	Total Courses	Total Credits
1	C	*COMPULSORY*	4	12
2	E	*ELECTIVES*	4	12
3	NG	*Non-Graded*	2	0
4	T	Thesis	**2 (16+16) + 8**	32+8
		Total		**64**

*for Direct students and students with different background.

Program compulsory (C)	Electives (E)
Thermodynamics of Materials *Characterization of Materials* *Symmetry, Structure and Tensor Properties* *Functional Materials*	Any from the Elective list

Department of Materials Engineering

Program Name M.Tech. Materials Engineering (Specialization in Functional Materials)

1. The following four courses are compulsory for M.Tech. students of the department:

S.No.	Course Number	*Course Title*	L-T-P	Credits
1	MTL7XX0	*Thermodynamics of Materials* (existing course)	2-0-2	3
2	MTL7XX0	*Characterization of Materials* (existing course)	2-0-2	3
3	MTL7XX0	*Symmetry, Structure and Tensor Properties* (existing course)	3-0-0	3
4	MTL7XX0	*Functional Materials* (existing course)	3-0-0	3

2.M.Tech. students shall have the option to choose four courses from the following list of courses:

Electives

S.No.	Course Number	*Course Title*		
1	MTL7XX0	Advanced Transmission Electron Microscopy (existing)	2-0-2	3
2	MTL7XX0	Functional 2D Materials (existing)	2-0-2	3
3	MTL7XX0	Materials for Electrochemical Energy Conversion and Storage (existing)	3-0-0	3
4	MTL7XX0	Processing and Engineering Application of Magnetic Materials (existing)	3-0-0	3
5	MTL7XX0	Processing of Polymer Matrix Composites (existing)	2-0-0	2
6	MTL7XX0	*Computational Modelling in Materials Engineering* (existing)	2-0-2	3
7	MTL7XX0	*Machine Learning for Materials Design* (existing)	2-0-2	3
8	MTL7XX0	Fundamental of Scintillation Detector Materials (existing)	3-0-0	3
9	MTL7XX0	Advanced Semiconductor Materials and Device Applications (existing)	2-0-2	3
10	MTL7XX0	*Advanced Molecular Dynamics* (existing)	3-0-0	3
11	MTL7XX0	Fundamentals and applications of battery materials (existing)	3-0-0	3
12	MTL7XX0	Solar Cell Materials and Devices (existing)	3-0-0	3

DETAILED SYLLABUS FOR CORE COURSES

Title	**Thermodynamics of Materials**	**Number**	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	2–0–2 [3]
Offered for	M.Tech.	Type	Compulsory
Pre-requisite			

Objectives

Provide a basis for describing and understanding the stability of various forms of matter.
Provide a basis for predicting the properties of an equilibrated system as a function of its content and characteristics.

Learning Outcomes

Understanding of the conditions for stability of a material and derive its properties.
Knowledge of parameters to control the evolution of microstructures.

Course Content

Laws of thermodynamics and Chemical reactions (13 lectures): First, second and third laws (3 lectures), statistical interpretation of entropy (3 lectures), Free energy functions and criteria for equilibrium (3 lectures), reaction equilibrium, equilibrium constant; applications to materials and metallurgical systems (4 lectures).
Thermodynamics of solutions and phase diagrams (13 lectures): Ideal and non-ideal solutions, partial and molar quantities, quasi-chemical model and regular solutions (3 lectures), Phase rule and binary phase diagrams (2 lectures), free energy composition diagrams (4 lectures), phase equilibrium calculations. (4 lectures)

***Laboratory Exercises*:**

1. Single-Point Equilibrium calculations
2. Calculation of thermodynamic properties of elements
3. Calculation Thermodynamic Properties of Compounds
4. Calculation Thermodynamic Properties of Solution Phases
5. Computation of Phase equilibria
6. Stepping in Temperature in the Fe-C System,
7. Fe-C Phase Diagrams calculations,
8. Fe-Cr-C Ternary Phase Diagram at 1000 K,
9. Stable and the Metastable Fe-C Phase Diagrams
10. Thermodynamics of reactions
11. Calculation of activation energy
12. Calculation of partition coefficient

Text Books

Gaskell, D.R., *Introduction to Metallurgical Thermodynamics*, McGraw-Hill 1995.
Swalin, R. A., *Thermodynamics of Solids*, reprint Edition, Wiley, 1962.
Saunders, N., Miodownik, A. CALPHAD (Calculation of Phase Diagrams): A Comprehensive Guide. United Kingdom: Elsevier Science, 1998.

Self-Learning Material

Hillert, M., *Phase Equilibria, Phase Diagrams and Phase Transformations Their Thermodynamic Basis,* Second edition, Cambridge University Press 2008.

Title	**Characterization of Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	2–0–2 [3]
Offered for	M.Tech.	Type	Compulsory
Pre-requisite			

Objective
Understanding the principles of instruments and methods for characterising different materials and their properties.

Learning Outcomes
Basic working knowledge of various instruments.
Ability to identify and choose different characterization techniques for specific property analysis.

Course Content
Structure of Materials (7 Lectures): Crystal structure, Symmetry elements, Miller indices, Stereographic projections, Reciprocal space, Structural characterization by X-ray diffraction, small angle scattering
Scanning electron microscopy (6 Lectures): Sample-electron interaction, Basis of image contrast and various operating modes, Low voltage SEM. Electron back scattered diffraction/OIM, micro-textural analysis.
Transmission electron microscope (6 Lectures): Lens defects, Mass-thickness contrast and diffraction contrast, Bright Field and Dark Field imaging, Electron Diffraction: SADP, Phase contrast and HRTEM.
Spectroscopic Characterization (7 Lectures): Optical emission spectroscopy, Energy dispersive spectroscopy, Electron Probe Microanalysis, Electron energy loss spectroscopy, X-ray fluorescence spectroscopy, X-ray photoelectron spectroscopy, FTIR, and Raman spectroscopy.

Lab Experiments
XRD Pattern Indexing;
XRD Profile fitting;
Lattice parameter and crystallite size calculation;
SEM/EDS analysis;
Orientation analysis using SEM-EBSD
Electron Diffraction Pattern Indexing;
Image Analysis;
UV-visible analysis and band gap calculation;
Functional group analysis using FTIR;
Calculation of thermodynamic parameters using DSC analysis;

Text Books
Zhang, S., Li, L. and Kumar, A., *Materials Characterization Techniques*, CRC Press, 2008.
Brandon D., Kaplan W.D., Microstructural Characterization of Materials, 2nd Edition, Wiley, 2008
Barrett C. S., Massalski T. B., Structure of Metals. 3rd revised edition. Pergamon Press, 2006

Self-Learning Material
1. Evans, C., Brundle. R. and Wilson, *Encyclopaedia of Materials Characterization: Surfaces, Interfaces, Thin Films (Materials Characterization Series),* Butterworth-Heinemann, 1992.
2. Kaufmann, E.N., *Characterization of Materials, 3 Volume Set, 2nd Edition,* Wiley, 2012.

Online Course Material
Shankaran, S., Materials Characterization, Department of Metallurgical & Materials Engineering, Indian Institute of Technology, Madras, NPTEL http://nptel.ac.in/courses/113106034/
Biswas, K. and Gurao, N.P., Advanced Characterization Techniques, Department of Materials Science and Engineering, Indian Institute of Technology, Kanpur, NPTEL http://nptel.ac.in/courses/113104004

Title	**Symmetry, Structure and Tensor Properties**	**Number**	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3–0–0 [3]
Offered for	M.Tech.	Type	Compulsory
Pre-requisite	Linear Algebra and Matrix Mathematics, MATLAB/Mathematica		

Objectives
1. Introduce the concept of symmetry in crystal lattices, point groups, and space groups.
2. Use of symmetry in the tensor representation of crystal properties, including anisotropy, representation surfaces, elasticity, and applications to piezoelectricity.

Learning Outcomes
The students will be able to:
1. Learn how to calculate different thermodynamic properties of different materials.
2. Understand how crystalline anisotropy affects/governs the property anisotropy.

Contents
Introduction: Spherical trigonometry and Applications in crystallography. *(4 lectures)*

Crystal lattices: Direct lattice, Crystal systems, Bravais lattice. *(2 lectures)*

Point groups: Stereographic projection, Proper cubic point groups, Improper point groups (dihedral angle, inversion symmetry), Types of point groups: 2D and 3D lattices. *(7 lectures)*

Space groups: Enumeration of the operations, Different space groups with specific materials examples. *(6 lectures)*

Group theory: Basic Concepts, Character Tables, Examples, Symmetry and Lattice Vibrations: Mode of Vibrations, Jahn-Teller Effect. *(7 lectures)*

Tensor properties of materials: Basic tensorial operations, Transformation of axis, Eulerian angles, Orthogonality Neumann principle, Pseudo tensors, Symmetry and Mathematical properties of tensors. *(7 lectures)*

Different ordered tensors: 2nd order (Stress-Strain, Permittivity, Permeability, Thermal Expansion), 3rd order (Piezoelectricity), 4th order (Elasticity Tensor). *(6 lectures)*

Textbook
1.Newnham, R.E., *Structure-property relations* (Vol. 2). Springer Science & Business Media, 2012.
2. Nye, J.F., *Physical properties of crystals: their representation by tensors and matrices*. Oxford university press, 1985.

Reference Books
1. Buerger, M.J., *Elementary crystallography*, John Wiley & Sons, 1956.
2. International Tables for Crystallography Volume A: Space-group symmetry, ISBN: 978-0-470-68575-4.

Online Course Material
1. Wuensch, B., *Symmetry, Structure, and Tensor Properties of Materials*, DMSE MIT, MIT OCW, https://ocw.mit.edu/courses/materials-science-and-engineering/3-60-symmetry-structure-and-tensor-properties-of-materials-fall-2005/syllabus/.

Title	**Functional Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3-0-0 [3]
Offered for	M.Tech.	Type	Compulsory
Pre-requisite			

Objectives
1. To provide the students with a detailed understanding (synthesis/growth, structure, and properties) of the functional materials.
2. To develop an understanding of the usage of functional materials as a component of modern devices.

Learning Outcomes
The students will be able to:
1. Compare, correlate and investigate the different synthesis, characterization, and application of exemplar functional materials.
2. Integrate the understanding of functional materials' properties and their applications.

Contents
Material synthesis and processing of functional materials: Bulk Synthesis: Solid state synthesis, Sol-Gel synthesis, Thin-Film synthesis: Sputtering, Molecular beam epitaxy, CVD, 3D printing, electrospinning. *(7 lectures)*

Defects in solids: Defect types and dimensionality effect on defects, Characterization (morphological and spectroscopic), Control of defects. *(7 lectures)*

Semiconductor materials: Band structure, Doping, Band-Gap engineering. *(2 lectures)*

Applications: Beyond Si semiconductors, GaN, GaAs, SiC, Ga_2O_3, LEDs, and photovoltaic cells (CdS, CIGS, CZTS, Perovskites and Organic solar cell materials). *(6 lectures)*

Materials for energy applications: Thermoelectric materials: ZT value, Band-Gap, Conductivity engineering, Oxide materials, Heusler alloys, Artificial and hierarchical materials, Peltier cooling, Thermoelectric generator, , Dielectric, Piezoelectric, Ferroelectric materials and applications, *(7 lectures)*

Magnetic materials & applications: Magnetic exchange energy, anisotropy energy, Magnetic domains, Application of soft and hard magnetic materials, Magnetic data storage, Superconductors in electronics. *(6 lectures)*

Optical materials: Optical lithography, and applications, Electro-optic materials. *(4 lectures)*

Textbook
1. Askeland, D.R., Phule, P.P., Wright, W.J., *The Science and Engineering of Materials*, 6th edition, Cengage Learning, 2010.
2. Callister, W.D., Rethwisch, D.G., *Materials science and Engineering: An Introduction*, 8th edition, Wiley, 2010.
3. Mitchell, B.S., *An Introduction to Materials Engineering and Science for Chemical and Materials Engineers*, 1st ed., Wiley- Interscience, 2003.
4. Kittel, C., *Introduction to Solid State Physics*, 8th edition, Wiley, 2005.

Reference Books
1. Kasap, S.O., *Principles of Electronic Materials and Devices*, 3rd edition, McGraw-Hill, 2006.
2. Raghavan, V., *Materials Science & Engineering: A first course*, 5th edition, PHI Learning, 2004.

Online Course Material
1. Haridoss, P., *Physics of Materials*, NPTEL Course Material, Department of Metallurgy & Material Science, Indian Institute of Technology Madras, https://nptel.ac.in/courses/113/106/113106039/.

2. Garg, A., *Electroceramics*, NPTEL Course Material, Department of Material Science & Engineering, Indian Institute of Technology Kanpur, https://nptel.ac.in/courses/113/104/113104005/.

DETAILED SYLLABUS FOR ELECTIVE COURSES

Title	**Advanced Transmission Electron Microscopy**	Number	MTL7XXX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	2–0–2 [3]
Offered for	M.Tech., PhD	Type	Elective
Pre-requisite			

Objectives

1. Introduce the working principle of Transmission Electron Microscopy (TEM).
2. Introduce of advanced TEM techniques to understand the material characterization at the atomic scale.

Learning Outcomes

The students will be able to:

1. Develop an understanding of TEM from an experimental and theoretical perspective.
2. The basic and advanced TEM simulation techniques for atomic-scale High Resolution (Scanning/TEM) imaging.

Contents

Introduction of advanced techniques in TEM: Aberration correction in TEM, Z & Phase contrast, High angle annular dark field imaging, Electron Magnetic Circular Dichroism (EMCD). (*4 lectures*)

4D-Scannning Transmission Electron Microscopy (4D-STEM), Electron Energy Loss Spectroscopy (EELS). (*3 lectures*)

Cryo-Electron microscopy, Electron tomography, Lorentz microscopy, Holography in TEM, Differential phase contrast. (6 *lectures*)

Computational aspect of advanced TEM techniques: Multislice simulation of high-resolution TEM imaging, Phase and Z contrast imaging. (*4 lectures*)

Simulation methods for advanced TEM techniques e.g., EMLD, EMCD, 4D-STEM, EELS. (*3 lectures*)

Advanced concept of digital micrograph scripting, Simulation of differential phase contrast imaging, EELS data processing and analysis in TEM (6 *lectures*)

TEM simulation

1) Indexing of electron diffraction pattern.
2) Simulation of electron diffraction pattern.
3) Simulation of High-Resolution (HR-TEM) images.
4) Simulation of Scanning Transmission Electron Microscope (STEM) images in TEM.
5) Simulation of Electron Energy Loss Spectroscopy (EELS) spectra.
6) Basics of digital micrograph scripting (installation and environment setting).
7) Processing HR-TEM images by digital micrograph scripting.
8) Processing EELS, STEM image data by digital micrograph scripting.

Textbook

1. Kirkland, E.J., *Advanced computing in electron microscopy*, Springer, ISBN:978-1-4419-6533-2, 2020.
2. Landup, D., *Data visualization in python with pandas and matplotlib*, ISBN:13: 979-8521342877, 2020.

Reference Books

1. Brent, F., James, H., Transmission Electron Microscopy and Diffractometry of Materials. Springer, Berlin. ISBN 978-3-642-29760-1 (2013).

Title	**Functional 2D Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	2–0–2 [3]
Offered for	M.Tech., PhD	Type	Elective
Pre-requisite			

Objectives

1. To introduce the emergent field of functional 2D materials.
2. Provides a comprehensive overview of 2D materials their hybrids and heterostructures systems that are relevant to different scientific applications.

Learning Outcomes

Upon completion, students are expected to

1. To know the basics of 2D materials.
2. Van der Waal and Non- van der Waal materials hybrids and heterostructures.
3. Design and fabricate 2D Advanced Materials based devices.

Contents

Fundamentals of 2D Materials

Introduction of functional quantum materials, 2D family, Electronic, Magnetic, Optical properties of functional quantum materials, Dirac metals, Weyl fermions. *(5 lectures)*

2D functional quantum materials at atomic scale, Topological insulators, Computation of electronic properties of functional quantum materials, Investigation of defect and Ohmic/Schottky contacts. *(4 lectures)*

Fundamental and properties of two-dimensional materials in sensing: Introduction, Band Alignment, Parameters of sensor performance. *(4 lectures)*

Fabrication of Devices, Application and Challenges

Synthesis (top-down and bottom-up approach and challenges), Characterization, and transfer of Van der Waals (graphene, boron nitride, Molybdenum disulphide, Tungsten Disulphide, Black Phosphorus, etc.) atomic sheets, Microscopic characterization by TEM. *(3 lectures)*

Non-Van der Waals Materials (Borophene, Hematene, Plumbene, MXene, etc.) their Hybrids (2D/1D, 2D/2D, 2D/3D), composites and heterostructures, Fabrication of 2D Material devices and challenges. *(3 lectures)*

Application of 2D Materials and their hybrids as well as heterostructures: Introduction (Graphene, Xenes, MXene, and Complex 2D Materials) Opto-Electronics (LEDs), Gas Sensor, Bio-Sensor, Drug-Delivery, Filtration/Desalination, Photovoltaics, Energy Storage and Generation, Lubricants, Environmental Remediation. *(5 lectures)*

Challenges with 2D Materials hybrids/heterostructures and device fabrications. *(2 lectures)*

Lab:

1) Synthesis of Van der Waals 2D material (e.g. Graphene, TMDCs) atomic sheets.
2) Characterization (morphological and spectroscopic) of the atomic sheets.
3) Fabrication of nano-devices (bio sensors, gas sensors, etc.).
4) Failure analysis and Quality control.
5) Synthesis of non-Van der Waals 2D material (e.g. Hematene, borophene, etc.) atomic sheets.
6) Characterization (morphological and spectroscopic) of the atomic sheets.
7) Fabrication of nano-devices (bio sensors, gas sensors, etc.).
8) Failure analysis and Quality control.

9) Synthesis of 2D hybrids and heterostructres (e.g. graphene/graphene oxide/reduced graphene oxide/borophene/hematene/TMDCs, etc.) atomic sheets.
10) Characterization (morphological and spectroscopic) of the atomic sheets.
11) Failure analysis and Quality control.

Textbook

1. Zettilli, N., Gubernatis, J.E., Lookman, T., *Quantum Mechanics: Concepts and Applications, Wiley*, 2009.

2. Griffiths, D.J., *Introduction to quantum mechanics*, Prentice Hall International, 2004.
3. Banks, C., E., Browson, D.A.C., *2D Materials, Characterization, Production and Applications*, CRC Press, 2017.

Reference Books

1. Ng, L.W.T., Hu, G., Howe, R.C.T., Zhu, X., Yang, Z., Jones, C., Hasan, T., *Printing of Graphene and Related 2D Materials: Technology, Formulation and Applications*, Springer, 2019.
2. Errana, G., *Metal Oxide Nanostructures as Gas Sensing Devices,* CRC Press, 2012.
3. Avouris, P., Heinz, T.F., Low, T.*, 2D Materials Properties and Devices*, Cambridge University Press, 2017.

References

1. Paglione, J., Butch, N.P., Rodriguez, E. E., *Fundamentals of Quantum Materials: A Practical Guide to Synthesis and Exploration,* World Scientific Pub Co Inc, 2021.
2. Heitmann, D., Quantum Materials, *Lateral Semiconductor Nanostructures, Hybrid Systems and Nanocrystals,* Springer, 2010.
3. Bartolomeo, D., *2D Materials and Van der Waals Heterostructures,* MDPI, ISBN 978-3-03928-769-7, https://doi.org/10.3390/books978-3-03928-769-7.
4. Hywel, M., Rout, C.S., Late, D.J., *Late Fundamentals and Sensing Applications of 2D Materials,* Elsevier, 2021.

Title	**Materials for Electrochemical Energy Conversion and Storage**	Number	MTL7XX0
Department	Metallurgical and Materials Engg.	L-T-P [C]	3-0-0 [3]
Offered for	B.Tech. final year, M.Sc., M.Tech., Ph.D.	Type	Elective
Pre-requisite			

Objectives
The instructor will:
1. Provide the student with the basic principles and recent advances in Energy Storage & Conversion materials for consumer electronics to high-power applications.
2. Provide the students with the Energy Storage & Conversion devices

Learning Outcomes
The students are expected to gain knowledge on:
1. Different modes of energy conversion, and storage.
2. Structure processing property performance relationship of energy materials

Contents

Introduction ***(4 lectures)*****:** Overview of electrochemical energy storage and conversion devices, Classification, Applications.

Capacitors ***(4 lectures)*****:** Concept, fundamental principles, various types, materials development, ceramic, polymer and electrolytic capacitors, applications, introduction to supercapacitors

Supercapacitors (Ultracapacitors) ***(2 lectures)*****:** Concept and working principles, Development of electrolyte and electrode materials, carbon-based nanomaterials, Transition metal dichalcogenides (TMDs), applications and challenges.

Batteries ***(6 lectures)*****:** Introduction to batteries, Concept of primary and secondary batteries, Lead acid, Nickel cadmium/MH and Li-ion batteries, Cell voltage, capacity and energy, Phase diagram and charge discharge, Metal-air, all liquid and flow batteries. Batteries for portable electronics, electric vehicles and grid storage

Supercapacitors (Pseudocapacitors) ***(3 lectures)*****:** Ultracapacitors *and* pseudocapacitors, faradaic charge storage in capacitors like batteries. Development of metal oxides, hybrid capacitors

Solar cells ***(2 lectures)*****:** Introduction, working principle, electrochemical Dye synthesized solar cells, Fabrication of devices

Solar fuel ***(3 lectures)*****:** Concept and overview, Photochemical, photobiological, electrochemical and thermochemical methods, Photo electrolysis

Fuel cells ***(6 lectures)*****:** Principle and types, Performance characteristics and Efficiency of fuel cells, Materials aspects, challenges and benefits, Proton exchange fuel cells, Solid oxide fuel cells: High and Intermediate temperature, Single chamber solid oxide fuel cells, Polymer electrolyte fuel cells, Acid/alkaline fuel cells, Phosphoric acid fuel cells, Molten carbonate fuel cells, Fuel cell stack

Electrochemical characterizations ***(3 lectures)*****:** IV curve, polarization and EIS for supercapacitors and batteries

Hydrogen Production & Storage ***(6 lectures)*****:** The Steam Reforming Process, Thermal Decomposition, Chemical extraction from Water, Electrolytic Production; Hydrogen Storage

High-Pressure Tanks, Metal Hydrides, Ammonia and Related Materials

Textbook

1. Cheong, K.Y., Impellizzeri G., Fraga M.A., *Emerging Materials for Energy Conversion and Storage*, 1st Edition, Elsevier, 2018.

Reference Books

1. Rosen, M. A., *Energy Storage*, Nova, 2012.
2. Electrochemical Methods: Fundamentals and Applications, Prof. Allen J. Bard and Larry R. Faulkner, WILEY, ISBN: 978-0-471-04372-0, December 2000, 864 pages

Online Course Materials

1. Bazant, M., MIT open course ware: Electrochemical Energy Systems, MIT Course Number 10.626/10.426, https://ocw.mit.edu/courses/chemical-engineering/10-626-electrochemical-energy-systems- spring-2014/.
2. Pal, K., *Selection of Nanomaterials for Energy Harvesting and Storage Application*, NPTEL Course Material, Mechanical Engineering, Indian Institute of Technology Roorkee, https://nptel.ac.in/courses/112/107/112107283/.

Title	**Processing and Engineering application of Magnetic Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering and Physics	L–T–P [C]	3–0–0 [3]
Offered for	M.Tech., PhD	Type	Elective
Pre-requisite	Basic knowledge of Quantum Mechanics		

Objectives

1. The course will provide knowledge of the underlying phenomena of magnetism.
2. Emphasis will be on the preparation process & characterization methods of magnetic materials used for engineering applications.

Learning Outcomes

The students are expected to have:

1. The ability to understand magnetic phenomena, and the metallurgical aspect of developing magnetic materials.
2. They will also get exposure to the engineering application of magnetic methods and magnetic materials.

Contents

Fractal-1: Fundamentals of Magnetism

Origin of magnetism, Bohr magnetron, Magnetic field and their calculation, Susceptibility and Permeability, Energy associated with the magnetic field, Thermodynamics of magnetic field, Magnetic forces, Spin orbit coupling, Crystal field. *(4 lectures)*

Classification of magnetic materials, Weiss molecular field, Exchange interaction, Magnetic anisotropy, Domains, Domain wall and domain wall motion, Magnetic hysteresis and Barkhausen emissions, Techniques for characterization of magnetic materials, Magnetic transport property, Magnetostriction, Magnetocaloric effect. *(9 lectures)*

Fractal-2: Processing and application of Soft and Hard Magnetic Materials

Nickel Iron alloys, Cobalt-Iron alloys, Electrical steel (CRNO, CRGO), Rapid solidification and amorphous electrical steel, Amorphous & Nanostructured magnetic alloys, Soft ferrites, Microstructure and magnetic property co-relations. *(5 lectures)*

Hard Magnetic Materials: Alnico, NdFeB, SmCo, MnBi, Hard ferrites. *(5 lectures)*

Heusler alloys and their applications. *(3 lectures)*

Fractal-3: Processing and application of Magnetic thin films and nanomaterials

Deposition of magnetic thin films and multilayers, Magnetic energy of thin film materials, Characterisation of magnetic thin films. *(3 lectures)*

Magnetic coupling in thin films, spin valve structure, Giant magneto resistance and tunneling magneto resistance, sensors. *(4 lectures)*

Magnetic wires and needles, Magnetic nanoparticles, Superparamagnetism, Quantum dots and molecular magnets, 2-D magnets. *(3 lectures)*

Application of magnetic nanomaterials in Biology and sustainable technology. *(3 lectures)*

Textbook

1. Chen, C.W., *Magnetism and Metallurgy of Soft Magnetic Materials* (Dover Books on Physics), Courier Corporation, 2013.
2. Cullity, B.D., Graham, C.D., *Introduction to Magnetic Materials*, 2nd Edition, Wiley, 2009.
3. Coey, J.M.D., *Magnetism and Magnetic Materials*, Cambridge University Press, 2010.

Reference Books

1. Jiles, D., *Introduction to magnetism and magnetic materials*, Chapman and Hall, 1991.
2. Chikazumi, S., *Physics of Ferromagnetism*, 2nd Edition, OUP Oxford, 2009.

Title	**Processing of Polymer Matrix Composites**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	2-0-0 [2]
Offered for	MTech	Type	Elective
Prerequisite	Polymer courses in UG level, Manufacturing processes		

Objectives

1. The main objective of the course is to impart an understanding of the processing of polymers and polymer composites such as Extrusion, Injection molding, Thermoforming, Compression molding and Transfer molding.

Learning Outcomes

1. Upon completion of this course, a student should be exposed to processing techniques of polymer and polymer composites.

Contents

Fractal 1

Introduction: [4 lectures] Engineering materials and processing techniques, Thermoplastics and thermosets, Processing of polymers, Composite materials: basic concepts, Classification of composite materials.

Processing of polymer composites: [9 lectures] Hand-layup, Spray-layup, Compression molding Injection molding. Reaction injection molding, Autoclaving, Resin transfer molding, Filament winding, Pultrusion. Sheet molding, Pre-pegging and challenges in primary processing of composites.

Fractal 2

Detailed processing techniques: [6 lectures] Thermoforming process. Extrusion, Transfer molding, Rotational molding, Blow molding.

Secondary processing of polymer composites: [7 lectures] Joining of polymer composites, Adhesive joining. Mechanical joining, Microwave joining, Induction and resistance welding, Drilling of polymer composites.

Laboratory Experiments

NA

Textbook

1. Mallick, P. K., *Processing of Polymer Matrix Composites: Processing and Applications*, CRC Press, 2018
2. Debnath, K. and Singh, I., *Primary and Secondary Manufacturing of Polymer Matrix Composites*, CRC Press, 2018.

Reference Book

1. Osswald T. A., Ortiz J. P. H. (2006), Polymer Processing Modeling and Simulation, Hanser
2. Agassant J. F., Avenas P., Sergent J. P. and Carreau P. J. (1991), Polymer processing: Principles and modeling, Wiley

Online Course Material

1. Prof. Inderdeep Singh, Processing of Polymers abmnd Polymer Composites, NPTEL Course Material, Dept. of Mechanical & Industrial Engineering, IIT Roorkee, https://nptel.ac.in/courses/112/107/112107221/
2.

Course Title	**Computational Modelling in Materials Engineering**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L–T–P: C	2–0–2 [3]
Offered for	M.Tech.	Type	Elective
Pre-requisite			

Objectives

1. Introduce first-principles calculations and molecular dynamics.
2. Introduce crystal plasticity and phase-field modelling techniques.
3. To provide hands-on experience in using computer simulation tools for studying materials.

Learning Outcomes

1. Able to use quantum and atomistic simulation tools
2. Awareness of modelling techniques at different length scales
3. Familiarity with the advantages and limitations of computational tools available for studying materials.

Course Content

First-principles calculations (7 lectures): Introduction, Periodic Structures, Supercells, Electronic kinetic energy cut-off, Total Energy, Geometry Optimization, Electronic Structure and Magnetic Properties, Calculations for Surfaces, Defects in solids.

Molecular dynamics simulations (7 lectures): Introduction, Application of various distribution functions in amorphous and crystalline materials, Study of Diffusion and activation energy barrier, Application of MD in studying the kinetics of battery electrodes and electrolytes, Steered molecular dynamics: Theory and application.

Phase-Field Modelling (6 lectures): Microstructure evolution, Continuum vs sharp interface description, The Ginzburg-Landau free energy functional, Equilibrium interfaces and surface tension, Conserved and non-conserved order parameters, Driving forces, fluxes, Spinodal decomposition in a binary alloy.

Introduction to Crystal Plasticity (6 lectures): Deformation gradient and finite strain, rotation and stretch, elastoplastic decomposition, Flow rules, hardening rules, slip systems and resolved shear stress, Pole figures and stereographic projection, Phenomenological models, dislocation-based constitutive laws.

Computer Simulations

1. Calculation of the electronic band structure and density of states in a semiconductor
2. Calculation of the electronic band structure and density of states in a metal
3. Calculate glass transition temp of polymer
4. Yield mechanism of an Au nanowire
5. Determination of the elastic stiffness tensor
6. Spinodal decomposition in a binary alloy
7. Modeling of grain growth:
8. Generation of synthetic 3D polycrystalline grain structure from Electron Backscatter Diffraction (EBSD) data
9. Simulation of uniaxial compressive stress-strain response of a polycrystalline FCC single-phase metal based on strain rate-independent and strain rate-dependent 3D Crystal Plasticity constitutive laws
10. Materials data visualization

Text Books

1. Lee, J., Computational Materials Science: An Introduction, 2nd Edition, CRC Press 2016.
2. Sholl, D. S., and Steckel, J. A., Density Functional Theory: A Practical Introduction, 1st Edition, Wiley, 2009.
3. Provatas, N., Elder, K., Phase-Field Methods in Materials Science and Engineering, John Wiley & Sons, 2011.
4. Roters, F., Eisenlohr,P., Bieler, T., Raabe, D., Crystal Plasticity Finite Element Methods in Materials Science and Engineering, WILEY-VCH Verlag GmbH & Co. KGaA, 2010.
5. LeSar, Richard, Introduction to Computational Materials Science: Fundamentals to Applications, Cambridge University Press, 2013.

References:

1. Raabe, D., Computational Materials Science: The Simulation of Materials, Microstructures and Properties, Wiley VCH, 1998.

2. Hull, D., and Bacon, D. J., Introduction to Dislocations, Butterworth-Heinemann (Elsevier), 5th Ed., 2011.

Online Course Materials:

1. MIT open courseware: Gerbrand Ceder, and Nicola Marzari. 3.320 Atomistic Computer Modeling of Materials (SMA 5107). Spring 2005. Massachusetts Institute of Technology: MIT OpenCourseWare, https://ocw.mit.edu. License: Creative Commons BY-NC-SA

2. Voorhees, P.W., Phase Field methods: From fundamentals to applications, Department of Material Science and Engineering, Northwestern University,
https://www.youtube.com/watch?v=FTiBq1o-8e4

Title	**Machine Learning for Materials Design**	Number	7XX0
Department	Metallurgical and Materials Engineering	L–T–P: C	2–0–2 [3]
Offered for	M.Tech.	Type	Elective
Pre-requisite	-		

Objectives

1. Introduce a selected set of Machine learning and Deep Learning techniques for Materials design.
2. Introduce hands-on experience with some practical methods and techniques in materials informatics for materials classification, regression, clustering, and adaptive design.
3. Introduce hands-on experience in analyzing data and applying ML approaches through a set of case studies pertaining to Materials Engineering.

Learning Outcomes

1. Aware of different data-driven techniques for creating Materials Knowledge.
2. To use machine learning tools for solving problems in materials design

Course Content

Deep Learning Techniques:
Supervised Learning using deep networks: Convolutional Neural Networks (CNN), Recurrent Neural Networks (RNNs), Self-Supervised Learning, Few Shot Learning, adversarial Learning, and Transformers. (13 lectures)

Unsupervised Learning using deep networks: Auto encoders, Deep Belief Networks (5 lectures)

Ensemble Classifiers: Random Forests, Gradient Boosted Decision Trees (4 lectures)

Association Analysis: Mining association rules, Graph Neural Networks (4 lectures)

Laboratory exercises:

1. A deep-learning technique for phase identification using synthetic XRD powder patterns
2. Physics-driven ML for catalysts design
3. Data-Driven Prediction of Interatomic Potentials
4. Automated Micrograph Analysis: Optical, SEM, TEM and EBSD analysis.
5. Data-Driven Approach for design and rapid screening of High Entropy and Amorphous alloys
6. Materials Property Predictions Based on Data from Chemistry, Structure and Processing
7. Data Driven Modelling for Defect prediction during Additive Manufacturing Process
8. Fatigue life prediction using ML

Books

1. Pilania, G., Balachandran, P. V., Gubernatis, J. E., and Lookman, T., *Data-Based Methods for Materials Design and Discovery: Basic Ideas and General Methods*, Morgan & Claypool Publishers, 2020.

2. *Machine Learning And Data Mining In Materials Science*, Edited by Huber, N., Kalidindi, S. R., Klusemann, B. and Cyron, C. J., Frontiers in Materials, 2020.

3. Mueller, T., Kusne, A.G. and Ramprasad, R., *Machine Learning in Materials Science.* In Reviews in Computational Chemistry, Edited by Parrill, A.L., and Lipkowitz, K.B., John Wiley & Sons, 2016.

Reference Books:

1. *Materials Informatics: Methods, Tools, and Applications*, Edited by Olexandr Isayev, Alexander Tropsha, Stefano Curtarolo, John Wiley & Sons, 2019

2. *Informatics for Materials Science and Engineering-Data-driven Discovery for Accelerated Experimentation and Application*, Edited by: Krishna Rajan, Butterworth-Heinemann, 2013

Title	**Fundamental of Scintillation Detector Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3-0-0 [3]
Offered for	M.Tech, PhD	Type	Elective
Pre-requisite			

Objectives

1. A fundamental understanding of various scintillation detectors materials, and their characteristics.

Learning Outcomes

Upon completion students are expected to

1. Get a general overview of scintillation detectors
2. Have an insight into the scintillator material composition, critical elements, and usage.

Contents

Introduction, Scintillation detector basics, Components of a scintillation detector, Detection efficiency – Density factor, Detection efficiency –Thickness Factor, Total detection efficiency, Energy transfer/interaction in scintillating materials, Properties of ideal scintillation materials. Cross scintillation mechanism, Organic scintillators– Liquid organic, Plastic, Loaded organic, Response of organic scintillators. *(13 lectures)*

Inorganic scintillators – Scintillation mechanism, Glass scintillators, Scintillator gases, Radiation damage effects in inorganic scintillators, Nanoscintillator – Structural effect, Surface effect, dielectric confinement, Form of nanoscintillators – Nanoparticles, Thin-Films, Nano-Ceramics. Photomultiplier tubes and photodiodes: Photocathodes – Photoemission, Spontaneous electron emission, Spectral response, Fabrication, Statistics of electron multiplication, Photomultiplier tube characteristics, Silicon photo multiplier. *(13 lectures)*

Photodiodes – Advantages, Conventional, Avalanche, Charge coupled devices, Radiation spectroscopy with scintillators: General considerations in gamma ray spectroscopy, Properties of scintillation gamma ray spectrometers, Characterization of scintillating materials, customizing scintillation detector – Tradeoffs on materials, Sizes and Components, Specialized detector configurations based on scintillation – Phoswich detector, Moxon-Rae detector, Position sensitive scintillators. *(13 lectures)*

Textbook

1. Knoll, G.F., *Radiation and Detection,* 4^{th} edition, ISBN: 0470131489, 2010.

Reference Books

1. Korzhik, M., Gektin, A., *Engineering of Scintillation Materials and Radiation Technologies: Proceedings of ISMART*, Springer, ISBN: 978-3-319-68465-9, 2016.
2. Yanagida, T., *Inorganic scintillating materials and scintillation detectors*, Proc Jpn Acad Ser B Phys Biol Sci. 9, 94(2): 75–97. Doi: 10.2183/pjab.94.007, 2018.
3. Duclos, S., *Ceramic Scintillators*, Annual Review of Materials Science, 27, 69-88, 1997.

Title	**Advanced Semiconductor Materials and Device Applications**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering and Electrical Engineering	L-T-P [C]	2-0-2 [3]
Offered for	M.Tech./Ph.D.	Type	Elective
Pre-requisite			

Objectives
1. To develop an understanding of the layered and non-layered semiconductor materials synthesis/growth and characterization techniques used in the semiconductor industry.

Learning Outcomes
The students will be able to:
1. Understand the basics of advanced semiconductor materials properties, failure analysis methods, reliability, and characterization.
2. Fabricate semiconductor layered material devices and analyse their properties.

Contents
Fractal-1: Material Synthesis and Characterization

Introduction, Basics of semiconductor, Crystallographic properties of the semiconductors. *(7 lectures)*
Growth and synthesis of semiconductor materials (2D and 3D), Defects and its characterization and Advantages of 2D materials. *(6 lectures)*

Fractal-2: Device Characterization

Electrical characterization of semiconductors: Material influenced test structure based electrical characterization methods like: two-probe/four-probe, Van der Pauw method, Hall-effect measurements etc. *(5 lectures)*

Characterization of junctions and diodes: C-V measurements, Life-time measurement, Metal-semiconductor: Schottky contacts, Barrier-height measurement, I-t techniques. *(4 lectures)*

Reliability and failure analysis: Gate oxide reliability measurement, Time-to-breakdown and charge to breakdown and Failure analysis, Noise measurements and analysis. *(4 lectures)*

Lab:
1) Synthesis of semiconductor materials atomic sheets of Graphene Oxide (MT).
2) Synthesis of semiconductor elemental sheets of Xenes and Transition metal dichalcogenides (TMDCs) (MT).
3) Fabrication of p-n junction (Graphene/Si/SiO_2, G/MoS_2, etc.) (MT).
4) Characterization of p-n junction (Graphene/Si/SiO_2, G/MoS_2, etc.) (MT).
5) Electrical characterization of the fabricated devices (EE).
6) Reliability and Failure analysis (EE).
7) Material process (spectroscopic) and Quality control (MT).
8) Tailoring the electrical, optical and Youngs' modulus of the semiconducting materials (MT).
9) Application of semiconductor in sensing (SERS/gas/strain) (MT/EE).
10) Application of semiconductor in opto-electronics (MT/EE).

Textbook
1. Schroder, D.K., *Semiconductor Material and Device Characterization,* 3rd edition, Wiley-Interscience, New York, 2006.
2. Nicollian, E.H., Brews, J., *MOS Physics and Technology,* ISBN: 978-0-471-43079-7, 1982.

Online Course Material

1. Haridoss, P., *Physics of Materials*, NPTEL Course Material, Department of Metallurgy & Material Science, Indian Institute of Technology Madras, https://nptel.ac.in/courses/113/106/113106039/.
2. Parasuraman, S., *Fundamentals of electronic materials and devices*, NPTEL Course Material, Department of Metallurgy & Material Science, Indian Institute of Technology Madras, https://nptel.ac.in/courses/113/106/113106039/.

Title	**Advanced Molecular Dynamics**	Number	MTL7XXX0
Department	Metallurgical and Materials Engineering	L–T–P [C]	3–0–0 [3]
Offered for	M.Tech.	Type	Elective
Pre-requisite	--		

Objectives

1. The aim of this course is to provide the student with an understanding of the various molecular dynamic's methods, their capabilities, and their limitations.

Learning Outcomes

1. Make sound judgements regarding the quality of molecular simulation studies reported in the literature
2. Have exposure to various advanced molecular dynamics techniques to reach experimental level times scale
3. Get an idea to set up the molecular dynamics simulations to solve realistic problems

Course Content

Molecular dynamics of hard spheres, demonstrating elementary concepts of temperature, ensemble averaging, error estimation, periodic boundaries, classical potentials and Machine learning potential. Equations of motion, integration schemes, Various ensembles and their applications, dynamical properties-Macroscopic Transport Phenomena (10 Lectures)

Limitations of Equilibrium Methods, Non-Equilibrium Molecular Dynamics, One (Disfavored) Approach, Basic theory and example of static and dynamic linear response, Diffusion: An Inhomogeneous Approach, Self-Diffusion: Perturbation, Thermostatting, Shear Viscosity: Boundary-Driven Algorithm, Limitations of Boundary-Driven Shear (12 Lectures)

Accelerated molecular dynamics, Parallel-Replica Dynamics, Hyperdynamics, Temperature-Accelerated Dynamics, Recent Advances and Applications, Overview of sampling methods (5 Lectures)

Ab-initio molecular dynamics, Basics of Nonadiabatic molecular dynamics, Different flavors of nonadiabatic molecular dynamics (5 Lectures)

Overview of various software to perform molecular dynamics, A model example of molecular dynamics calculation and its result analysis. (7 Lectures)

Books

1. Allen, M.P. and Tildesley, D.J., *Computer Simulation of Liquids*, Clarendon Press, Oxford 1987.
2. Frenkel, D. and Smit, B., *Understanding Molecular Simulation*, second edition, Academic Press, San Diego, 2002.
3. Marx, D. and Hutter, J., *Ab Initio Molecular Dynamics*, Cambridge University Press, Cambridge, 2009.

References:

1. Hiroki Nakamura, *Introduction To Nonadiabatic Dynamics*, World Scientific Press, 2019, https://doi.org/10.1142/11359
2. *Ab Initio Nonadiabatic Quantum Molecular Dynamics*, Chem. Rev. 2018, 118, 7, 3305–3336.
3. *Annual Reports in Computational Chemistry*, Volume 5, 2009, Elsevier B.V., ISSN: 1574-1400, DOI 10.1016/S1574-1400(09)00504-0

Title	**Fundamentals and Applications of Battery Materials**	Number	MTL7XX0
Department	Metallurgical and Materials Engineering	L-T-P [C]	3-0-0 [3]
Offered for	B.Tech final year, MSc., M.Tech., Ph.D.	Type	Elective
Prerequisite	-		

Objectives
Through this course the instructor will provide an insight into the
1. Fundamentals of batteries and working principles
2. Development of battery materials and different battery technologies.

Learning Outcomes
The students are expected to gain knowledge on:
1. Selection of batteries depending on working conditions,
2. Roadmap to develop battery materials, role of electrodes, electrolytes and their interface
3. Electrochemical methods available to characterize battery materials

Contents

Fundamentals of Electrochemical Cells along with history and evolution of primary cells *[6 lectures]:* Chemical and Electrochemical Reactions, Concept of Voltaic cell, Operation of a Cell, Self-Discharge, Thermodynamic & kinetic parameters: Cell Voltage, Capacity, and Energy, Current, State of charge, Issues with Voltaic Cells, Development of Daniell cell, Zinc-air & Alkaline-MnO_2 cells.

Concept of rechargeable Cells *[6 lectures]:* Concept of electrochemical reversibility, attempts to develop rechargeable Cells, Concept of structural reversibility, Charge-discharge curves, Columbic efficiency, Development of Negative electrodes such as Zinc and Cadmium & Metal Hydrides, Development of Positive electrodes such as Manganese Dioxide/ The “Nickel” Electrode / Lead oxide. Insertion Reaction, Reconstitution Reaction

Lead-Acid Batteries *[3 lectures]:* Basic Chemistry, Voltage & SoC, Theoretical Specific Energy, Mechanisms of the Electrochemical Reactions in the Electrodes, Volume Changes and Shedding, VRLA batteries.

Batteries based on the “Nickel” Electrode *[4 lectures]:* Nickel-Iron Batteries, Nickel-Cadmium Batteries, Nickel-Zinc Batteries, Nickel-Hydrogen Batteries, Nickel-Metal Hydride Batteries

Li-ion batteries *[10 lectures]*: Concept and working principle, Negative Electrodes in Lithium Cells: Electrochemical Behaviour, structural reversibility, Amorphization, Decrepitation, Modifications, Positive electrodes with Layered, Spinel & Olivine Structure, Development of Electrolytes**,** Stability of Electrolytes Vs. Alkali Metals, Elevated Temperature Electrolytes for Alkali Metals, Electrolyte Stability Windows and Their Extension, Composite Structures that combine stability regimes, Solid electrolytes, Solid-state batteries

Batteries based on different Li-based chemistry *[3 lectures]:* Primary systems such as the Li/MnO_2, Li/SO_2 & $Li/SOCl_2$ System, Li-ion, Lipo, Sn/Co & Amprius batteries, NMC, LFP, LTO batteries

Batteries beyond Li-based chemistry *[3 lectures]*: Na/Al/Mg/Fe/V-ion batteries, Liquid metal batteries, Structural batteries

Battery Characteristics, Performance, Design, Selection & Standardization *[2 lectures]:* General Characteristics and Factors Affecting Battery Performance, Batteries of different shapes and sizes, Battery Design and Construction, Selection and Application of Batteries

Electrochemical Techniques for Characterization of Battery Materials ***[2 lectures]*:** Galvanostatic charge-discharge, differential capacity vs. Capacity plot, Impedance spectroscopy, Galvanostatic intermittent titration, Li+ transport number calculation, Application of AI & machine learning in designing and operating batteries.

Textbook

1. Huggins R. A. (2009) *Advanced Batteries: Materials Science Aspects*, 1st Edition, Springer

Reference Books

1. Linden D. and Reddy T. B. (2002) *Handbook of Batteries, 3rd Edition*, The McGraw-Hill Companies

Online Course Material

Prof. Bazant M., MITopencourseware: Electrochemical Energy Systems, MIT Course Number 10.626 / 10.426,
https://ocw.mit.edu/courses/chemical-engineering/10-626-electrochemical-energy-systems-spring-2014/

Title	**Solar Cell Materials and Devices**	Number	MTLXXXX
Department	Metallurgical and Materials Engineering	L-T-P	3-0-0 [3]
Offered for	UG/PG	Type	Elective
Prerequisite	Basic understanding of electronic materials/materials science		

Objectives
The course provides an understanding of the solar cell materials with the latest advancements, focusing on their properties, fabrication, characterization, and applications.

Learning Outcomes
The students are expected to **(i)** understand the fundamental properties of materials used in solar cells. **(ii)** Learn the solar cell fabrication processes and performance factors **(iii)** Analyze the structural, electrical, and optical properties of solar cell materials using relevant characterization techniques.

Contents

Introduction [4 lectures]: Photovoltaic (PV) Technology, Electromagnetic Radiation and Energy Harvesting, Energy Conversion Mechanisms in Solar Cells, Fundamental Limits to Photovoltaic Conversion.

Basics of Solar Cells [4 lectures]: Physics of p-n junction diode under dark and illumination, Solar Cell Equivalent Circuit, Characteristics of Solar Cells (V_{OC}, J_{SC}, FF, Efficiency, Series and Shunt Resistance), Types of Solar Cells, Light management in Solar cells.

Silicon based Solar Cells [6 lectures]**:** Introduction to Silicon Solar Cells, Monocrystalline Silicon Solar Cells, Polycrystalline Silicon Solar Cells, Amorphous Silicon Solar Cells, Fabrication Methods, Scope of Improvement.

III-V Solar Cells: Materials and Applications [5 lectures]**:** Homo and Hetero junction III-V Solar Cells, GaAs Solar Cells, InP Solar Cells, InGaAsP Solar Cells, GaN, Multijunction Solar Cells, Fabrication Methods.

Thin Film Solar Cells: [6 lectures]: Introduction and Advantages, Thin Film Solar Cell Materials - Binary and Quaternary Chalcogenides, Fabrication Methods.

Emerging Solar Cells [8 lectures]: Dye-sensitized solar cells, Perovskite solar cells, Organic Solar Cells, Hybrid Solar Cells, Quantum Dot and Nanostructured Solar Cells, Tandem Solar Cells, Bifacial Solar Cells.

Characterization and Simulation Studies [6 lectures]**:** Structural and Morphological Characterization, Optical (UV-Vis, PL and TRPL) and Electrical Characterization: Hall Effect and I-V Measurements, Case Studies on Simulation-Driven Performance Optimization of Solar Cells.

Textbooks:
1. Thomas Dittrich, Materials Concepts for Solar Cells, Imperial College Press, 2014.
2. Jenny Nelson, The Physics of Solar Cells, Imperial College Press, 2003
3. S.K. Sharma, K. Ali, Solar Cell from materials to device technology, Springer Nature, 2020.
4. J. Poortmans, and V. Arkhipov, Thin Film Solar Cells: Fabrication, Characterization, and Applications, Wiley, 2006.

Reference Books:
1. Laurentiu Fara, Masafumi Yamaguchi-Advanced Solar Cell Materials, Technology, Modeling, and Simulation, Engineering Science References, 2013.
2. Peter Würfel, Physics of Solar Cells: From Basic Principles to Advanced Concepts, Wiley-VCH, 2016.

Video link: NPTEL
NPTEL, Solar Photovoltaics: Principles Technologies and Materials
https://www.youtube.com/watch?v=Xcy6rTYxijQ
NPTEL-NOC IITM
(https://www.youtube.com/watch?v=tSD8lgdicNk)

NPTEL, Electronic materials, devices, and fabrication
https://www.youtube.com/watch?v=mCgXsEyQZSI