SS830 INTRODUCTION TO NANOCOMPOSITES 3-1-0-4

Introduction to Nanomaterials

Introduction to nanomaterial science, Interdisciplinary nature, Structure of nanomaterials, Length scales, de-Broglie wavelength &exciton Bohr radius, Fundamentals of Quantum Mechanics: wave function, Schrödinger equation, uncertainty principle, quantum wells, quantum dots, quantum wires.

Characterization techniques

Introduction to materials and characterization techniques; Spectroscopic methods-UV-Visible and vibrational spectroscopy- Infrared and Raman, Electron spectroscopies- X-ray photoelectron spectroscopy, Ultra-violet photoelectron spectroscopy, Auger electron spectroscopy; X-ray techniques- X-ray diffraction, X-ray fluorescence spectrometry; Optical microscopy, Electron microscopy- SEM, TEM; Scanning Probe microscopies- STM and AFM.

Nanocomposites

Introduction to Nanocomposites, Composite material, Mechanical properties of Nano composite material: stress - strain relationship, toughness, strength, plasticity. Introduction to Nanocomposites, Structure and Properties - Dispersion, Matrix Bonding, and Functionalization, matrix-nanomaterial interactions. Thin film nanocomposites; Modeling of nanocomposites.

Ceramic Matrix Nanocomposites (CMNC)

Mechanical alloying, thermal spray powder method; Polymer precursor route; Spray pyrolysis; Vapour techniques (CVD and PVD) and Chemical methods, which include the sol-gel process, colloidal and precipitation approaches and the template synthesis synthesis

Metal Matrix Nanocomposites (MMNC)

Spray pyrolysis; Liquid metal infiltration; Rapid solidification; Vapour techniques (PVD, CVD); Electrodeposition and Chemical methods, which include colloidal and sol-gel processes.

Polymer Matrix Nanocomposites (PMNC)

Nano coatings, Nano particle dispersion in polymer matrix-processing of polymer nano composites, processing of organic-inorganic hybrid materials. Intercalation of the polymer or pre-polymer from solution; In-situ intercalative polymerization; Melt intercalation; Direct mixture of polymer and particulates; Template synthesis; In-situ polymerization; Sol-gel process. Chemical and electrochemical methods.

TEXTBOOKS/ REFERENCES:

1. T. Pradeep, nano the essentials: UnderstandingNanoscience and Technolgy, McGraw-Hill professional publishing, 2008.
2. Charles P.Poole.Jr.& Frank J.ownes, Introduction to Nano technology - John wielly&sonsInc.Publishers -2006
3. Guozhong Cao, Nano structures and Nano materials: Synthesis, properties and applications, Imperial College press.
4. P.M. Ajayan, L.S. Schadler and P.V. Braun, Nanocomposite Science & Technology,- Wiley-VCH GmbH Co.
5. Z.L. Wang, Characterization of nanostructured materials
6. B. Roszek , The Handbook of Nanotechnology –Wiley, 2005
7. Nanomaterials, Nanotechnologies and Design: An Introduction for Engineers and Architects- Daniel L. Schodek, Paulo Ferreira, Michael F. Ashby (Butterworth - Heinemann)

8. Nanostructures and Nanomaterials: Synthesis, Properties, and Applications" (2 nd Edition) (World Scientific Series in Nanoscience and anotechnology) -Guozhong Cao and Ying Wang (Imperial College Press)

SS831 POLYMER TECHNOLOGY 3-1-0-4

Polymer processing

Processing methods for the manufacture of products with dry rubber, blending and mastication, master batching of of polymers, mixing and compounding in mills and internal mixers, calendaring, sheeting, fabric coating, extension, moulding. Batch curing methods: autoclave curing, gas curing, over curing, water curing, lead curing, cold curing. Processing methods for plastic products manufacture: methods of mixing, injection, compression and transfer moulding, extrusion, calendaring, thermoforming, blow moulding, rotational moulding and slush moulding.

Polymerization techniques

Bulk polymerization, solution polymerization, emulsion polymerization, suspension polymerization, interfacial polymerization, melt polycondensation, solution polycondensation, solid and gas phasepolymerization.

Polymer testing

Importance of standards and standard organisations. Processability and performance, testing of plastics and rubbers, material characterisation tests such as melt flow index, capillary rheometer test, viscosity test, gel permeation, chromatography, and thermal analysis.

Material characterisation tests for thermosets. Apparent bulk density, bulk factor and pourability of plastics materials. Flow tests such as spiral blow, cup flow, viscosity tests for thermoset resins bubble viscometer, Brookefield viscometer, gel time and peak exothermic temperature of thermosetting resins.

Polymer properties

Mechanical properties: Tensile strength, flexural and compression properties, creep properties, stress relaxation, impact properties, shear strength, abrasion, fatigue and hardness etc. Thermal properties: heat deflection temperature, vicat softening temperature, torsion pendulum test, thermal conductivity, thermal expansion, brittleness temperature.

Electrical properties; dielectric strength, dielectric constant, dissipation factor, electrical resistance, arc resistance etc. Weathering properties: UV, IR, X-ray, microorganisms, humidity, ozone oxygen, water, thermal energy, chemical factors.

Optical properties: Refractive indices, luminous transmittance and haze, colour, gloss.

Polymer characterisation

Functional group analysis, use of chemical reactions and degradation for structural analysis, various microscopic techniques such as light microscopy, electron microscopy etc. and spectroscopic techniques such as IR, FTIR, NMR,EPR,UV-Visible, Raman, fluorescence etc.

TEXTBOOKS/ REFERENCES:

1. J.A. Brydson, Plastics Materialsa,Butterworths,1989
2. F.W. Bilmer, Textbook of polymer science, Wiley interscience,1971
3. W.A. Holmes Walker, Polymer Conversion, Applied Sciences 1975
4. Maurice Morton, Rubber technology
5. M. Blow, Rubber Technology and Manufacture, Newness, Butterworths,1977
6. R.T Fenner, Principles of polymer processing, Macmillan,1979

SS832 POLYMER SCIENCE 3-1-0-4

Polymerisation mechanisms

Chemistry of condensation polymerisation, types of condensation polymers. Types of stepwise reactions. Interfacial condensation, Ring opening polymerisation reactivity and molecular size.

Poly functional condensation polymerisation gelation, gel point experimental observation, Molecular weight distribution, ring scission polymerisation, Metathesis polymerisation, group transfer polymerisation

Heat and free energy of polymerisation, Cationic polymerisation – mechanisms and kinetics of anionic polymerisation, examples, kinetics and mechanism, co-ordination polymerisation, polymerisation with supported metal oxides. Different types of catalysts, kinetics of step polymerisation, copolymerisation, and reactivity ratios.

Methods of polymerisation

Copolymerization: types of copolymers, the copolymer composition equation,monomer reactivity ratio and copolymer structure, influence of structural effectsof monomers on monomer reactivity ratios, the Q-e scheme, synthesis ofalternating, block and graft copolymers.Step reaction(condensation) polymerization-kinetics and mechanism of stepreaction polymerization, Carothers equation, number distribution and weightdistribution functions, polyfunctional step reaction polymerization, prediction of gel point. Controlled polymerization methods-nitroxide mediated polymerization, AtomTransfer Radical Polymerization(ATRP), Reversible Addition Fragmentation Termination(RAFT), electrochemical polymerization, metathetical polymerization, group transfer polymerization.

Polymer reactions

Hydrolysis, acidolysis, aminolysis, hydrogenation, addition and substitution reactions, Reaction of various specific groups, cyclisation reaction, cross linking reactions, reactions leading to graft and block copolymer.

Polymer viscoelasticity, introduction to the viscoelastic properties of polymers,some simple linear viscoelastic models-Maxwell model, Voigt model, seriescombination of Maxwell and Voigt model, generalized linear viscoelasticity, the Boltzman principle, the linear viscoelastic behavior of polymer solids, creepexperiments, stress relaxation experiments, stress-strain experiments, oscillatoryexperiments, the elastic modulus, time temperature equivalence, time-temperaturesuperposition principle.

Rheological properties of polymers-introduction to polymer melt rheology,Newtonian fluids, non-Newtonian fluids, pseudoplastic, thixotropy, St. Venantbody, dilatant, complex rheological fluids, rheopectic fluids, time dependentfluids, time independent fluids, power law, Weissenberg effect, laminar flow,turbulent flow, die swell, shark skin, viscous flow, melt flow index.Transport in polymers-diffusion, liquid and gas transport, Fick's law, theories ofdiffusion.

TEXTBOOKS/ REFERENCES:

1. F.W. Bilmeyer, Textbook of polymer science, Wiley Interscience,1971
2. H. R. Allock and F.W. Lampe, contemporary polymer chemistry, Prentice hall,1981
3. G. Odian, Principles of Polymerisation, McGraw Hill,1970
4. Polymer science and technology, Fried
5. Physical Chemistry of Macromolecules, Tanford, C. John Wiley,1961
6. P.J.flory, Principles of Polymer Chemistry, University Press, London, 1953

SS833 MATERIALS: FUNDAMENTAL SCIENCE AND ADVANCED APPLICATIONS
3-1-0-4

Introduction to Material Science

Material resources and their implications, Functional Classification of Materials, Trends in the periodic table, Inter-atomic bonding, intermolecular forces and bonding (Ionic, Covalent and Metallic Bonding), Concept of hybridization and basic understanding of molecular orbital theory,

Structure of materials:

1. Metals and Alloys (crystal structures and systems, important parameters in cubic space lattices, crystal locations planes and directions, interplanar spacings, Brags law, points defects, Hume–Rothery rules, line defects, planar defect)
2. Ceramics and Glasses- Pauling's Rules, ceramic crystal structure- rock salt, diamond structure and spinel structure, silicates and crystalline silicate networks, structure of glass, difference between glassy and amorphous solids, Zachariasen Rules, Stanworth Rules, Defect Reactions- Kroger–Vink Notation
3. Polymers- Functional groups in polymer chemistry, classification- thermoplastic and thermoset, tacticity, copolymers, degree of polymerization, Average molecular weight, types of bulk polymer Crystallinity, liquid crystalline polymers, glass transition
4. Composites- Composite Constituents and classification, combination effects, composite matrixes (Polymer metal ceramic), reinforced composites, particulate composites, composite interphase, functionally graded materials
5. Biologics- Amino acids, DNA & RNA, cells, hard and soft biologics

Environmental Impact on the structure property relationships in materials, Materials design and selection Thermal conductivity applied to metal, ceramics, polymers, semiconductors, Thermal shock Degradation and Failure of structural materials: Corrosion- Galvanic and single metal corrosion, role of Cl, H2 and NH3 in corrosion, control- passivation and design control, gaseous oxidation- Pilling-Bedworth ratio, wear-types, fracture- brittle and ductile fracture, Fatigue- cyclic stress and S-N curve, Factors that affect fatigue life.

Electron Microscopy

Limitations of the Human Eye, Properties of an Ideal Image, Imaging with Electrons, instumentation of TEM, iamging and vacumm system, TEM images- Electron-Electron Scattering, bright field and dark field images, electron diffraction patterns, TEM Specimen Preparation (Chemical , electrochemical, ion-beam and thin film deposition Thinning), Operating Principle of the SEM, Secondary-Electron Images, Backscattered-Electron Images, specimen-current image, EBIC image, CL images, SEM Specimen Preparation, The Environmental SEM, Electron-Beam Lithography, Analytical Electron Microscopy- X-Ray Energy-Dispersive Spectroscopy, Quantitative Analysis in SEM & TEM, X-Ray Wavelength-Dispersive Spectroscopy, Comparison of XEDS and XWDS Analysis, Auger Electron Spectroscopy, Electron Energy-Loss Spectroscopy, Scanning Transmission Electron Microscopy.

Electronic, Magnetic and Photonic Materials

Electrical conductivity of materials, band theory of solids, semiconductors (types and conductivity), insulators, conductivity of metals and alloys, deposition of thin films (PVD, sputtering, CVD, electrodeposition)

Classification and a brief overview of Diamagnetic, Paramagnetic, Ferromagnetic, Ferrimagnetic, and Super paramagnetic Materials, Curie temperature, Applications of magnetic materials, Magnetostriction

Electromagnetic spectrum, consequences of Refraction, Reflection, Absorption and Transmission, Emission phenomena (Gamma rays- nuclear interactions and X-rays—Inner Electron Shell Interactions), Luminescence—Outer Electron Shell Interactions, Light-Emitting Diodes—Electroluminescence, Lasers, Thermal Emission, Fiber optic communication systems

Materials in Medicine

Classes of materials used in medicine, steps in fabrication of metallic implants, microstructure and properties of stainless steels, cobalt based alloys, titanium based alloys, clinical applications and types of polymers used in medicine, properties of some important bio medically and pharmaceutically important hydrogels, bioresorable and bioerodible materials, biodegradation, bioerosion, bioabsorption and bioresorption as applicable to biomaterials, biodegradable polymers, bioceramic material, types of bioceramics-tissue attachment, porous ceramics, bioactive glasses and glass-ceramics, resorable calcium phosphates, applications of collagen based biomaterials, carbon and polymers fibers as reinforcing material, examples of surface modified biomaterials

Organic Photovoltaics and Electrochemistry

Relevance of Photovoltaics in the current energy scenario, renewable energy –merits and demerits, solar spectrum, solar cell- Shockley solar cell equation, electrical characteristics- (I-V), quantum efficiency, spectral response, Optical properties- Anti reflection coating, light trapping, silicon solar cell structure- p-n Junction Solar Cell, Heterojunction Cells, The p-i-n Structure, Series Resistance

Origins of Photoelectrochemistry, Organic Photovoltaic Materials, Principles of Operation and Device Concepts- Homojunctionsm, Heterojunctionsm, Dispersed Heterojunctions, Leading Device Designs (2000-2013), Challenges in Organic Photovoltaic materials and design, Organic Photovoitaic Modules

Fluorene-Containing Polymers for Solar Cell Applications- Bulk Heterojunctions, Polyfluorene-Containing Photovoltaics, Bulk Heterojunction Device Performance, Low-Band gap Materials,

Electrochemical Fluorination- Aromatic Rings, Olefins, Sulfides, Heterocyclic Compounds, Inorganic Fluoride Salts, and Benzylic Electrochemical Fluorination, commercialized Anodic fluorination and anodic methoxylation of ethyl phenylthioacetate

Electrochemical Polymerization- conditions

TEXT BOOKS/ REFERENCES:

1. Brian s. Mitchell, An Introduction to Materials Engineering and Science for Chemical and Materials Engineers, John Wiley & Sons, inc., Hoboken, New Jersey, 2004.

2. Donald R. Askeland, Pradeep P. Fulay and Wendelin J. Wright, The Science and Engineering of Materials, Sixth Edition, Cengage Learning, Inc, 2010

3. Milton Ohring, Engineering Materials Science, Academic Press, Inc, 1995.

4. William D. Callister, Jr. and David G. Rethwisch, Materials Science and Engineering- An Introduction, Eighth Edition, John Wiley & Sons, Inc, 2010.

5. Ray F. Egerton, Physical Principles of Electron Microscopy, Springer Science+Business Media, Inc, 2005

6. Buddy D Ratner and Allan S Hoffman (eds), Biomaterials Science, Academic Press, 1996
7. Konrad Mertens, Photovoltaics, John Wiley & Sons Ltd, 2014
8. Tom Markvart and Luis Castafier, Solar Cells: Materials, Manufacture and Operation, Elsevier Ltd, 2005
9. Toshio Fuchigami, Shinsuke Inagi, Mahito Atobe, Fundamentals and Applications of Organic Electrochemistry, John Wiley & Sons, Ltd, 2015
10. Christoph Brabec, Vladimir Dyakonov, and Ullrich Scherf, Organic Photovoltaics, WILEY-VCH Verlag GmbH & Co. KGaA, Weinheim, 2008

SS834 ORGANIC CHEMISTRY: STRATEGIES IN ORGANIC SYNTHESIS 3-1-0-4

i) Oxidations: Swern oxidation, Prevost oxidation and Woodward oxidations with detailed understanding of reaction mechanism and it's application.

ii) Reductions: Birch reduction, Reduction with $LiAlH_4$, $NaBH_4$, BH_3, AlH_3, and tri-n-butyl tin hydride.

iii) Organo- metallic reagents: Use of Organo lithium, Silicon and boron reagents in Organic synthesis.

iv) Modern Organic Synthetic Reactions: Aza-Cope and Aza-Wittig reactions, Baylis-Hillman reaction, BINAL and BINAP assisted reactions, Buchwald-Hartwig coupling, Click reaction, Grubb's catalyst and RCM olefin metathesis, Heck reaction, Julia- Lythgoe olefination, Mukayama aldol reaction, Mitsunobu reaction, McMurray reaction, Peterson's stereoselective olefination, Suziki, coupling.

v) Conducting polymers: Electrically conducting polymers and their uses (polyanilines, polypyrrole, polyacetylene and polythiophene). Photoconductive polymers. Liquid crystal polymers – smectic, nematic and cholesteric structures, Some important conductive polymers e.g. PEDOT-PSS.

TEXT BOOKS/ REFERENCES:

1. Some modern methods of organic synthesis by W Carruthers
2. Guidebook to organic synthesis, by R K Meckie, D M Smith & R A Atken
3. Organic synthesis by O House
4. Organic synthesis by Michael B Smith
5. Reagents for organic synthesis, by Fieser & Fieser, Vol 1-11(1984)
6. Organic synthesis by Robert E Ireland
7. Organic Synthesis - The disconnection approach by S Warren
8. Organic Synthesis by C Willis and M Willis
9. Handbook of reagents for organic synthesis by Reich and Rigby, Vo I, IV
10. Problems on organic synthesis by Stuart Warren
11. Total synthesis of natural products: the Chiron approach by S.Hanessian
12. Organic chemistry Claydon and others 2005
13. Name Reactions by Jie Jack Li
14. Reagents in Organic synthesis by B.P.Mundy and others.
15. Tandem Organic Reactions by Tse-Lok Ho
16. Textbook of Polymer Science, F. W. Billmeyer Jr, John Wiley & sons
17. Polymer Science, V. R. Gowarikar, N. V. Viswanathan & J. Sreedhar, Wiley Eastern
18. Contemporary Polymer Chemistry, H. R. Alcock & F. W. Lambe, Prentice Hall
19. Physics and Chemistry of Polymers, J. M. G. Cowie, Blackie Academic and professional
20. Ploymer Chemistry, B. Vollmert
21. Physical Chemistry of Polymers, A. Tagers, Mir Publishers
22. Introduction to polymer Chemistry, By Charles E Carraher Jr (Taylor- Frncis)
23. Much emphasis will be made on reports in current literature pertaining to Organic Synthesis.

The following references can be followed for general guidelines.

24. B.M. Trost (ed.) Comprehensive Organic Synthesis: Selectivity, Strategy and Efficiency in

Modern Organic Chemistry, Pergamon Press, Oxford, Vols 1-9, 1991.

25. E.J. Corey and X..-M.Cheng, The Logic of Chemical Synthesis, Wiley, New York, 1989.
26. J.D. Morrison (Series Ed.) Asymmetric Synthesis Academic Press, New York.

SS835 APPLICATION OF COMPUTATIONAL CHEMISTRY 3-1-0-4

1. Computational method I - Ab initio techniques –basis sets-inputing initial geometries (z-matrices and others), semiemperical methods – density functional theory – molecular mechanics
2. Computational method II - molecular dynamics – computing molecular geometries, potential energy surfaces, – molecular vibrations – population analysis – chemical properties by computational methods
3. Computational method III - Ab initio techniques – semiempeicl methods – density functional theory – molecular mechanics – molecular dynamics – computing molecular geometries, potential energy surfaces, Z matrices – basis sets – molecular vibrations – population analysis – chemical properties by computational methods
4. Computing the transition states, reaction co-ordinates, reaction rates, solvation, electronic excited states, structure property relations, computing NMR chemical shifts, Band structures, Meso scale dynamics, synthesis route prediction
5. Periodic table, Molecular modeling, modeling of biomolecules, simulating liquids, polymers, solids and surfaces the software packages.

TEXT BOOKS/ REFERENCES:

David C. Young, 'Computational Chemistry' 1st edition, Wiley-Interscience, 2001
Andrew R. Leach, 'Molecular Modeling – Principles and Applications', 2nd edition, Pearson Education EMA, 2001