Syllabus for courses in PSE division, CSIR-NCL, Pune

Course Title: Advanced Polymer Chemistry

Course Code: NCL205, Level: 200, Credits: 3

1. Introduction to Polymer Science: Brief history of plastics - Advantages and disadvantages - thermoplastics and thermosets. Manufacture of monomers - polymerization - structure - properties - processing and applications of some important industrial polymers.
2. Chemistry of Polymers: Concept of average molecular weight, Monomers, functionality, degree of polymerizations, classification of polymers, tacticity, glass transition, melting transition, criteria for rubberiness, polymerization methods: addition and condensation; copolymerization, random, alternating, techniques for copolymerization-bulk, solution, suspension, emulsion.
3. Polymer Characterization: Determination of molecular weights, (GPC, Viscosity) Thermal analysis techniques like DTA, DSC, TGA etc. Spectroscopic techniques like IR, UV, NMR etc. Application of these techniques to polymers.
4. Solution and Melt Processing of Polymers: Solubility of polymers, solubility parameters, good, bad and theta solvents: Melt processing of polymers, compression molding, injection molding, blow molding, extrusion, pultrusion, calendaring, rotational molding, thermoforming, rubber processing in two-roll mill, internal mixer.
5. Thermal Properties of Polymers: Glass and melt transition, locating the glass transition in polymers, free volume theory, factors that affect glass transition temperature, polymer crystallization, kinetics of nucleation and growth, lamellar and spherulite morphology, polymorphism and crystalline phase transitions
6. Polymer Conformations: Conformations, bond rotation and polymer size. Average end-end distance, Characteristic ratio, statistical segmental length, radius of gyration, self–avoiding chains
7. Viscoelastic Behavior of Polymers: Basic concepts: stress, strain, modulus, viscosity and compliance, viscous and elastic responses, stress relaxation and creep, Maxwell and Voight Model, entanglement and rubbery plateau, dependence of Me on molecular structure.
8. Polymer testing and specifications: Mechanical-static and dynamic tensile, flexural, compressive, abrasion, endurance, fatigue, hardness, tear, resilience, impact, toughness. Conductivity-thermal and electrical, dielectric constant, dissipation factor, power factor, electric resistance, surface resistivity, volume resistivity, swelling, ageing resistance, environmental stress cracking resistance.
Lab: a) Preparation of polymers i) Polymethylmethacrylate ii) Polystyrene, b) GPC c) Viscometry

References: 1) Experimental methods in polymer chemistry - Rabek, John Wiley & sons, New York, 1998
2) Industrial Polymers - Ulrich, Hanser Pub. Munich, N.Y.

Course Title: Modern Polymerization Methods for Functional Macromolecules

Course Code: NCL316, Level: 300, Credits: 2

1. Combination of mechanistically distinct polymerization techniques such as Atom Transfer Radical Polymerization (ATRP), Reversible Addition Chain Fragmentation Transfer (RAFT), Nitroxide Mediated Polymerization (NMP), Ring Opening Metathesis Polymerization (ROMP), Living ROP, Metal-Catalyzed Polymerization for sequential/tandem polymerization of various incompatible monomers, heterofunctional initiators, heterotelechelic polymers, functional polyolefins.
2. Incorporation of functionalities into polymers using Click Chemistry, for example azide-alkyne, thiol-ene, thiol-yne, thiol-bromide, thiol-disulfide exchange, nitroxide-radical, nitrile oxide-alkyne

addition, cycloaddition reactions, metal-free click chemistry, imine/hydrazone/oxime formation, photochemical conjugation.

3. Use of these click reactions in combination with above polymerization techniques for synthesis of functional macromolecular architectures such as block copolymers, star polymers, graft and brush copolymers, dendritic polymers, cyclic polymers, cyclic-linear copolymers. Polymer origami. Conjugation of biomacromolecules with polymers using click chemistry. Modular transformation of polymers.

4. Surface-initiated polymerization: Growing polymers/polymer brushes on surfaces to tune the surface properties of organic and inorganic materials, nanoparticles, nanoplatelets and nanorods. Different approaches such as *grafting to* and *grafting from* and the utilization of various modern polymerization techniques to create functionalized surfaces. Characterization methods and a wide range of applications for surface initiated polymerization.

Course Title: Polymer Physics

Course Code: NCL319, Level: 300, Credits: 2

What is a polymer? What is unique to polymers? Polymer characterization, including MW, MWD, Rg, Rh, intrinsic viscosity.

Models for flexible polymers. Random walk, self-avoiding random walk. Persistence length. Excluded volume interactions. Polymer solutions in the dilute limit/semi-dilute limit. Entropy of mixing, theta temperature, rubber elasticity: elasticity of a freely jointed chain,

Overview of polymer dynamics. Maxwell (phenomenological model). Bead-spring models. Reptation (scaling arguments).

Polyelectrolytes: Poisson Boltzmann/Debye-Huckel theory, Bjerrum length.

Polymer crystallization.

References: 1. Scaling Concepts in Polymer Physics by deGennes (Cornell Univ Press).
2. The Structure and Rheology of Complex Fluids by R. G. Larson (Oxford University Press).
3. Polymer Chemistry by P. C. Hiemenz and T. P. Lodge (CRC Press).

Course Title: Polymer Synthesis

Level: 300, Credits: 2

1. Introduction to polymers in general and classification in particular. Addition (chain) and condensation (step) polymerization with illustrative examples.

2. Radical chain polymerization, Rate of Radical Chain Polymerization, Initiation, propagation, Termination, Chain Transfer, Types of initiators, Autoacceleration, Molecular Weight Distribution, methods of polymerization, e.g. bulk, solution, suspension, emulsion, gas phase etc. Controlled or Living Radical Polymerization (CRP/LRP).

3. Ziegler-Natta polymerization, Coordination or insertion polymerization, Functional Olefin polymerization, Organometallic mediated polymerization; ROMP, ADMET, TEMPO-mediated polymerization and atom transfer radical Polymerization (ATRP).

4. Step-growth Polymerization, kinetics, molecular weight control in linear polymerization. Examples - polyesters, polyethers, polyamides, polyurethanes, polyurea, polycarbonate and other condensation polymers.

5. Cationic Polymerization and Anionic Polymerization, Applications of ionic polymerizations for synthesis of block copolymers, Ring opening polymerization

6. NMR and IR spectroscopy of polymers

Course Title: Polymer Characterization

Level: 200, Credits: 3

Characterization of polymers by up to fifteen methods including spectroscopic (nuclear magnetic resonance, Raman, infrared), mechanical (tensile, dynamic mechanical, rheological), microscopic (electron and optical microscopy), physiochemical (intrinsic viscosity, differential scanning, calorimetry, gel permeation chromatography) and scattering (light, x-rays).
Lectures will provide a state-of-the-art description of these and additional polymer characterization methods and also include hands-on training of some of the instruments used for polymer characterization.

Course Title: Polymer Processing and Rheology

Level: 300, Credits: 2

1. Theory of Rheology: Definitions of stress, strain, Ideal fluids and solids, Linear viscoelasticity (LVE), Introduction to non-linear viscoelasticity, Linking LVE to Molecular Weight Distribution (MWD), Introduction to mol. constitutive equations.
2. Rheometry: Controlled stress and controlled strain rheometers, Cone & plate and parallel plate geometries, Capillary rheometry, Extensional rheometry: uniaxial, biaxial, exponential shear, hyperbolic die, equibiaxial, Instabilities (slip, fracture, inertia).
3. Linking rheology to macromolecular architecture: Effect of MWD on rheology or determining MWD from rheology, Transformations of LVE data, Creep to G', G" and inverse, Stress relaxation to G', G" and inverse, Effect of long-chain branching (LCB) on rheology,
4. Lab sessions on rheometry, data interpretation and problem solving
5. Basics of various processing techniques: a) Extruders: single screw and twin-screw extruders, Film blowing, Fiber spinning, Pipe extrusion, Extrusion of profiles, Extrusion of cable material, Extrusion of sheet, Calendaring, and Thermoforming. b) One-dimensional process like Coating and Adhesives. c) Molding: injection molding, Compression molding, Transfer molding, Blow molding, Rotational molding, Gas and water assisted injection molding, Reaction injection molding, other three dimensional molding.
6. Compounding: Principles of polymer formulation and modification; Classification and type of Additive for Plastics; Classification and type of Fillers and Reinforcements for Plastics; Type of Impact Modifiers and their applications; Compounding processes and equipment; Use of experimental design in compound formulation; Masterbatch compounding.
7. Reactive Extrusion: Extruder as a reactor; Fit the reactor to Chemistry; Process analysis from reaction fundamentals; Type of Reactions; Process Considerations; Design of Reactive Extruder; and Devolatization.
8. Industry visit: Polymer Processing and other ancillary industries.

Course Title: Special Topics in Polymers

Level: 300, Credits: 3

1. Polymers in Healthcare:
a) Design and methods of synthesis of biocompatible and biodegradable polymers, Synthesis and characterization of drug conjugated polymers, Synthesis and characterization of polymer micelle and vesicles, Drug nanoparticles and drug containing nanofibers for biomedical applications, Pharmacokinetic study, *In-vitro* and *in-vivo* study.
b) Synthetic and Natural Polymers, blends, composites in medical devices, Physical and Chemical Properties of biomedical polymers and their characterization, Processing techniques to prepare

scaffolds, implants, micro/nanoparticles, Cell and biomaterial interactions and applications and examples.

2. <u>Water soluble polymers and Gels:</u> Introduction to water-soluble polymers and applications, Synthetic methodologies, Structure-property relationship, Associating polymers (APs)/Hydrophobically Modified Polymers(HMPs),clarification behaviour-by solution Rheology, Preparations, properties and applications of hydrogels.

3. <u>Membranes</u>: Basic introduction to membranes and membrane based processes, Mechanism of separation in various types of membrane processes, Application of different polymers as membrane materials.

4. <u>Polymers in energy:</u> Design and methods of synthesis of polymers for energy applications, Tools and methods to characterize conjugated polymers, Fabrication and characterization of devices for energy conversion

5. <u>Composite Materials:</u> Scope and general characteristics of composites; a broad perspective on various applications, Characteristics of fibers, matrices, interface bonding, adhesives; microstructure of composites; types of composites, Physico-mechanical properties of conventional fiber and particulate polymer composites, Traditional and novel approaches; process fundamentals, Basic concepts, stiffness, strength, thermal and moisture expansion, Failure criteria, Laminate Strength, Stress Concentrations, How do actual composites for aerospace, automotive, sporting goods, high temperature applications behave? Problem areas, long-term performance, Synthesis, characterization and application of polymer nanocomposites. Recent advancements, Design concepts; small group design problem using composites (design, build, and test)

4. <u>Microencapsulation:</u> Basics of Control Release Technology, Control Release forms: microcapsules, microspheres, Characterization, Applications