METALLOCENE AND METAL-CARBENE BASED ORGANOMETALLIC COMPOUNDS AS INDUSTRIALLY IMPORTANT ADVANCED POLYOLEFIN CATALYSTS

PROF. SANJIB K. PATRA
Department of Chemistry
IIT Kharagpur

PRE-REQUISITES : Basic organometallic chemistry

INTENDED AUDIENCE : UG, PG, PhD students; Relevant industrial persons

INDUSTRY SUPPORT : Polymer manufacturing industries

COURSE OUTLINE :

Among the various organometallic catalysts, metallocene and metal-carbene based catalysts have rapidly been developed for industrial use in olefin polymerization in the last two decades. The unique design, structural parameters and symmetry of metallocene catalysts afford exceptional activity in α-olefin polymerization in presence of activator to produce high molecular weight polyolefin where stereoregularity/microstructure can be finely controlled to meet the targeted applications. In parallel, the transition metal
carbene/alkylidene complexes with M=C bond have attracted chemists and industries as living alkene metathesis polymerization catalysts. In this course, the main focus will be to address the understanding the concept, designing principle of catalysts, reactions mechanism and developing pathways of these type of popular and attractive catalysts used in polymer industries. The knowledge gained in this course will further help to design and develop appropriate catalyst systems to achieve tailored polymers, oligomers and other value added compounds.

ABOUT INSTRUCTOR :

Prof. Sanjib K. Patra completed his Ph.D. in organometallic chemistry in 2007 from Dept. of Chemistry, IIT Kanpur. After that, he did his postdoctoral research as Marie Curie Postdoctoral Research Fellow in Prof. Ian Manners' group at University of Bristol (UK). Subsequently (Dec, 2011), he joined as assistant professor at Dept. of Chemistry, IIT Kharagpur. Currently, he is associate professor at IIT Kharagpur. The area of his research is interdisciplinary in nature comprising the fields of synthetic inorganic, organometallic, polymer and materials chemistry. The main interest of research is on synthesis and characterization of multifunctional materials. He teaches Inorganic, Organometallic, Polymer Chemistry, and Catalysis to UG/ PG/PhD students at IIT Kharagpur.

COURSE PLAN :

Week 1: A brief overview of transition metal/organometallic catalysts in industrially important processes with special focus on polyolefin industrial synthesis. Introduction to the most attractive class of catalysts based on Metallocene and Metal-carbene compounds; Structural variation with metal ions and ligands.
Week 2: Metallocene compounds: Synthesis, structural parameters, bonding, unique properties and reactivity; Evaluation of metallocene (Group 4 metals) catalysts in olefin polymerization.
Week 3: Understanding the polymerization mechanism; Choice and role of co-catalysts (aluminium and boron based); Strategic development of metallocene catalysts for tailored and high molecular weight LDPE, LLDPE, ethylene-α-olefin copolymers; Superiority over Ziegler-Natta catalysts.
Week 4: Controlling stereoregularity in polyolefin by Zr(IV)-metallocene catalysts: Designing and choice of ligands; Metallocene symmetry; Catalysts site control and chain end control mechanism; Correlation between symmetry of metallocene and stereo-regularity/microstructure/physical properties of the polyolefin.
Week 5: Supported metallocene catalysts for commercial process; Ti(IV) based constrained geometry catalysts for high molecular weight polyolefin: design, structure and mechanism; A brief discussion on dual role of metallocene catalysts in depolymerization - a highly demanding aspect at current time.
Week 6: Metal-carbene and alkylidene complexes - a unique class of organometallic compounds with M=C bond: Synthesis, structure, bonding, unique properties and reactivity.
Week 7: Metathesis reaction by metal carbene /alkylidene complexes (Ti, Mo, W, Ta, Ru) with special focus on ring-opening metathesis polymerization (ROMP) of cyclic olefins by Shrock's and Grubbs' catalysts; Concept and mechanism of polymerization.
Week 8: Discussion on development of living ROMP by Grubbs catalyst through a systematic approach; Role of ligands; Versatility of Grubbs' catalysts and compatibility towards functional groups and ring-strain of monomer; Well-defined copolymers by Grubbs' catalyst and industrial importance.