Programme: M. Sc. Part-II (Chemistry)
Course Code: PCO-502
Title of the Course: Catalysis: Fundamentals and Applications
Number of Credits: 03 **Effective from AY:** 2019-20

Prerequisites for the course:	Students should have studied the course PCC 401, PCO 401 in Semester I/II, so as to have basic knowledge of material chemistry and reaction kinetics.	No. of lectures/hours
Course Objectives:	1. To introduce concepts of surface science and catalysis 2. To provide fundamental knowledge of theories that govern heterogeneous catalytic reactions 3. To introduce newer methods of synthesizing nanocatalyst, porous catalyst and its characterization. 4. To introduce latest developments about application of catalyst in environment and energy sector.	
Course Outcomes:	1. Students should be in a position to understand the concept of heterogeneous surface science. 2. Students should be able to understand methods of synthesizing nano catalyst, tailoring morphological and chemical properties of the catalyst and its characterization. 3. Students should be in a position to understand and apply their knowledge in surface catalysed reaction of industrial and environmental significance.	
Content:	**1. Basic Concepts:** 1.1 General Introduction: Catalysis and activation energy. Homogeneous and heterogeneous reactions with suitable illustrations. Catalytic activity, selectivity and stability. Steps in a heterogeneous catalytic reaction. Factors affecting rate of reaction such as temperature, flow rates, molar composition etc. 1.2 Adsorption and Surface Area: Cause of adsorption. No of molecules striking the surface and sticking probability. Adsorption isotherms for gases and solutes. Basic types of BET isotherms. Chemisorption of H_2, O_2 and CO. Surface area and Porosity: Determination of surface area. Porosity and pore size distribution. 1.3 Classification of catalysts based on electrical conduction. Adsorption on specific crystal planes; geometric factor in catalysis: Balandin's multiplet theory and Valence angle conservation. Electronic effect in catalysis by metals. Role of diffusion in catalysis. **2. Kinetics and mechanisms of catalysed reactions** 2.1 Kinetics of catalysed reactions and rate expressions. Mechanism of catalysed reactions obeying Langmuir-Hinshelwood, Eley- Rideal and Mars van Krevelen models with suitable examples. **3. Preparation of Catalysts** 3.1 Various methods for preparation of bulk catalysts:	13 hours 6 hours 3 hours

	Precipitation method, Impregnation method catalyst impregnation with or without interaction between support and catalyst. Synthesis of microporous solids. Synthesis of mesoporous solids. 4. **Thermal and Spectroscopic Methods in Heterogeneous Catalysis** 4.1 Characterization of the catalysts by temperature programmed desorption using probes such as ammonia and pyridine molecules. Characterization of adsorbed molecules /intermediates by IR spectroscopy and XPS. **5. Selected Catalytic Applications** 5.1 Introduction to zeolites, structure building in zeolites with suitable example. Zeolite catalysis in MTG process. Introduction to semi-conductor surface and electrocatalysis with application in photocatalytic and electrocatalytic water splitting and treatment of waste water contaminated with dyes	4 hours 10 hours
Pedagogy:	Mainly lectures, tutorials, assignments, self-study or a combination of some of these could also be used to some extent.	
Text Books / Reference Books	1. D. K. Chakrabarty & B. Viswanathan, *Heterogeneous Catalysis,* New Age International Publishers, 2008. 2. G. A. Somorjai, *Introduction to Surface Chemistry and Catalysis,* John Wiley, 2002 3. M. Thomas & W. J. Thomas, *Principles and Practice of Heterogeneous Catalysis*, VCH Publishers, 1996.	