Name of the Programme: M.Sc. Part-II (Physical Chemistry)

Course Code: CHP-602 **Title of the course:** Heterogeneous Catalysis: Fundamentals and Applications

Number of Credits: 4

Effective from AY: 2023-24

Prerequisites for the course:	Students should have studied Chemistry courses at MSc Part-I.	
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 nanocatalysts and its characterization. 4. To introduce latest developments about application of catalyst in environment and energy sector.	
Concepts	1. **Basic Concepts** a. General Introduction: Catalysis and activation energy. 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. b. Adsorption and Surface Area: Cause of adsorption. No of molecules striking the surface and sticking probability. Types of adsorption and potential energy profiles for adsorption of H_2. Adsorption isotherms for gases and solutes. Basic types of BET isotherms. Gibbs adsorption equation and changes in surface tension. Free energy, enthalpy and entropy of adsorption. Chemisorption of H_2, O_2 and CO. Surface area and Porosity: Determination of surface area. Porosity and pore size distribution. c. Classification of catalysts based on electrical conduction. Adsorption on specific crystal planes; geometric factor in catalysis: Balandin's multiplet theory and Valence angle conservation. Cumulative & depletive adsorption, Electronic effect in catalysis by metals. Role of diffusion in catalysis.	No of hours 20
	2. **Kinetics and mechanisms of catalyzed reactions** Kinetics of catalyzed reactions and rate expressions. Mechanism of catalyzed reactions obeying Langmuir-Hinshelwood, Eley- Rideal and Mars van Krevelen models with suitable examples.	5

	3. **Preparation of Catalysts** Various methods for preparation of bulk catalysts: Precipitation method, Impregnation method catalyst impregnation with or without interaction between support and catalyst. Synthesis of microporous solids. Synthesis of mesoporous solids.	5
	4. **Thermal and Spectroscopic Methods in Heterogeneous Catalysis** Characterization of the catalysts by temperature programmed desorption using probes such as ammonia and pyridine molecules. Characterization of surface area using BET method. Characterization of adsorbed molecules/intermediates by IR spectroscopy and XPS. Introduction to EXAFS and Mössbauer spectroscopy in characterizing catalysts.	10
	5. **Zeolite based Catalysis and industrial applications** Structure building in zeolites such ZSM-5. Nature of active sites and their characterization. Role of Zeolite acidity and Shape Selectivity in catalytic reactions. Zeolite based catalysis in MTG process.	5
	6. **Semiconductor catalysis and its application in energy and environmental sector** Introduction to semi-conductor surface and catalysis with application in photocatalytic water splitting and CO_2 reduction to value added chemicals. Case studies on photocatalytic degradation of dyes. Practical demonstration of photocatalytic treatment of laboratory waste water contaminated with dyes, adsorptive separation and kinetic analysis.	10
	7. **Electrocatalysis and applications** Basic electro-catalytic concepts, comparison of electro-catalysts. Electrocatalytic water splitting reaction. Role of catalytic materials in energy storage applications.	5
Pedagogy:	Mainly lectures, tutorials, assignments, demonstration, self-study or a combination of some of these could also be used to some extent.	
Reference / Readings:	1. D. K. Chakrabarty and 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 and W. J. Thomas, Principles and Practice of Heterogeneous Catalysis, VCH Publishers, 1996. 4. P.P. Morajkar, A. P. Naik, S. T. Bugde, B. R. Naik, CH-20:	

	Photocatalytic and microbial degradation of Amaranth dye, Advances in Biological Science Research-A Practical Approach 2019, 327-345, Academic Press. 5. B.H.R. Suryanto, Y. Wang, R. K. Hocking, Overall electrochemical splitting of water at the heterogeneous interface of nickel and iron oxide. Nature Commun. 2019, 10, 5599. 6. A. V. Salkar; S. V. Bhosale; P. P. Morajkar, CH-6: Nanostructured WO_{3-x} Based Advanced Supercapacitors for Sustainable Energy Applications, Advances in Metal Oxides and Their Composites for Emerging Applications; Elsevier, 2022, 213–238. ELSEVIER. 7. A.V. Salker, Catalysis: Principles and Basic Concepts, Scientific International, 2019.
Course Outcomes:	1. Students will be able to design a nanocatalysts for adsorption application. 2. Students will be able to interpret characterization data of nano catalysts. 3. Students will be able to design a catalyst for environmental and energy applications. 4. Students will learn about semiconductor catalysis.