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

**Course Code:** CHI-602 **Title of the course:** Principles and applications in catalysis

**Number of Credits:** 4

**Effective from AY:** 2023-24

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| **Prerequisites for the course:** | Students should have studied chemistry courses at M.Sc. Part-I. | |
| **Course Objective:** | 1. To understand the fundamentals concepts of chemical reactions over the catalysts.<br>2. To understand energy saving and making green processes in chemical reactions.<br>3. To understand fundamentals and basic concepts of chemical reactions for developing higher productivity and viability.<br>4. To provide knowledge on applications of heterogeneous, homogenous and other catalytic processes.<br>5. To make aware of catalytic approaches in environmental pollution control processes. | |
| **Content** | **1. Origin and development of catalysts**<br>a. Introduction to heterogeneous, homogeneous and bio-catalysis, importance of catalysis in chemical reactions and its industrial applications.<br>b. Concepts of Atom Economy, Turnover number and Turnover frequency. | No of hours<br><br>5 |
| | **2. Heterogeneous Catalysis**<br>a. Introduction to heterogeneous catalysis, energy profile diagram and diffusion of gas, general mechanisms such as Langmuir-Hinshelwood and Rideal-Eiley.<br>b. Adsorptions: Physical and chemical adsorption, chemisorptions of gases on solid surfaces, nature of adsorbed layer, dissociative adsorptions, scattering, trapping and sticking, simple adsorptions isotherm, Langmuir adsorption, the BET adsorption isotherm and Surface area determination.<br>c. Types of Catalysts: Preparations and separations of the catalysts, meso and micro porous materials, nano material catalysts and significance, zeolites and related molecular sieves, supported and bifunctional catalysts and catalyst regeneration, activity and life of the catalysts, active centers, promoters and poisons, catalyst deactivations.<br>d. Characterization of solid catalysts: Structure and surface morphology, porosity, pore volume and diameter, particle size, X-ray diffraction , Thermal analysis (DTA/TG and DSC), SEM, TEM, X-ray absorption spectroscopy, XPS and Auger Electron Spectroscopy to surface studies, TPD for acidity and basicity of | 23 |

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| | the catalysts.<br>e. Heterogeneous reactions: Thermodynamic consideration in surface reactions, mechanism of catalytic reactions, ammonia synthesis, oxidation reduction reactions, CO oxidation, $N_2O$ decomposition, Fisher tropsch catalysis, selective catalytic reduction, method of finding reaction rate and the rate determining steps.<br>f. Theories of Catalysis: Boundary layer theory, catalysis by semiconductors, Wolkenstein theory, Balanding's approach, electronic factors in catalysis by metals, molecular orbital approach. | |
| | **3. Homogeneous Catalysis**<br>a. Homogeneous catalytic reactions, merits and demerits, intermediate stages in homogenous catalysis, energy profile diagram, activation energy, general scheme for calculating kinetics of the reactions.<br>b. Decomposition of hydrogen peroxide, acid-base catalysis.<br>c. Homogeneous catalytic reactions: Hydrogenation, hydroformylation, isomerization, Monsanto acetic acid process, Carboxylation reactions, Wacker reaction, coupling reactions and asymmetric oxidations. | 12 |
| | **4. Photo-catalysis**<br>Homogeneous photo-catalysis, photo-sensitized and photo-oxidations reactions, heterogeneous photo-catalysis, semiconductor photo-catalysts, generation of hydrogen by photo-catalysts and harnessing solar energy, photo-degradation of dyes. | 3 |
| | **5. Catalytic polymerizations**<br>Homogeneous and heterogeneous catalysis in polymerizations reactions (few examples), Ziegler – Natta catalyst in polymerizations reactions. | 5 |
| | **6. Bio-catalysis**<br>Nomenclature and classification of enzymes, metal ions and metalloenzymes, general properties, enzymatic reactions such as redox and decomposition, action of enzymes, mechanistic pathways of few enzymatic reaction, factors affecting enzymes and enzyme applications. | 3 |
| | **7. Phase transfer catalysis**<br>Mechanism of PTC, types of phase transfer catalysis with selected examples, advantages and disadvantage. | 3 |
| | **8. Catalyst for energy and environment**<br>Catalytic gasification, electricity from gas turbine, steam reforming, electro-catalysis, fuel cells for energy production like methanol, molten carbonate and solid oxide fuel cells, catalysts for environmental pollution in emission control and selective catalytic | 6 |

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| | reduction. | |
| **Pedagogy** | Mainly lectures and tutorials. Seminars / term papers /assignments / presentations / self-study or a combination of some of these can also be used. ICT mode should be preferred. Sessions should be interactive in nature to enable peer group learning. | |
| **References / Readings** | 1. A.V. Salker, Catalysis: Principles and Basic Concepts, Scientific International, 2019.<br>2. P. H. Emmett, Catalysis, Vol I, Reinhold,1955.<br>3. D. K. Chakraborty, Adsorption and Catalysis by Solids, New Age International (P) Ltd., 2008.<br>4. J. M. Thomas, W.J. Thomas, Heterogeneous Catalysis, VCH publication, 1997.<br>5. A. Clark, The Theory of Adsorption and Catalysis, Academic Press, 1970.<br>6. E. R. Rideal, Concept in Catalysis, Academic Press, 1968.<br>7. G. M. Panchenov, V. P. Lebedev, Chemical Kinetics and Catalysis, Mir publication, 1976.<br>8. S. J. Thomson, G. Webb, Heterogeneous Catalysis, Oliver and Boyd Publications, 1968.<br>9. R. A. Van Santen, J. W. Niemantsvedict, Chemical Kinetics and Catalysis, Plenum Press, 1995<br>10. M. Beller, A. Renken, R. van Santen, Catalysis, Wiley VCH, 2012. | |
| **Course Outcome:** | 1. Students will be able to explain concepts and general properties of different types of catalysts.<br>2. Students will be able to explain the catalytic reaction mechanisms and green catalytic processes.<br>3. Students will be in position to prepare and characterized catalysts.<br>4. Students will apply knowledge to develop reaction specific catalysts using basic concepts.<br>5. Students will apply knowledge to develop catalysts for useful chemical reactions and environmental pollution control processes. | |