Course No.	Course Name	L-T-P-Credits
CY 531	**Chemical Kinetics, Reaction and Molecular Dynamics**	**3-0-0: 03**
Prerequisite: NIL		

Course Objectives: The main objective of the course is to provide basic knowledge of kinetics of chemical reactions. The course targets to explain the different types of reactions and their kinetics in terms of rate laws. The objectives also lie to derive and understand the theories of chemical kinetics to obtain rate coefficient of chemical reactions, differences between gas phase and solution phase reactions, experimental methods to carry out fast reactions. The objective of the course is also to introduce the basics molecular dynamics in terms of equation-of-motion, force field, trajectory calculations, etc.

Course Outcomes: After successful completion of the course, students will be able to:

1. Learn about the fundamental concepts of obtaining rate laws for different order reactions
2. Understand the basic ideas different types of reactions and their kinetics
3. Learn the approximated methods to deal with complicated reactions
4. Understand the basic chemistry of reaction dynamics based on Potential Energy Surfaces (PESs)
5. Understand the factors that can affect the rate of a reaction in solution phase
6. Learn how fast reactions are tackled in different novel experimental techniques
7. Learn the basics of molecular dynamics and research domains in this field.
8. Engage themselves in the research domain of finding probable reaction path for a chemical reaction based on the theories explained in the course

SYLLABUS

Module	Contents	Hours
I	**Chemical Kinetics** Rate of reactions, kinetics and mechanism, rate laws, elementary reactions, consecutive reactions, steady state approximation, kinetic isotope effect, chain reactions, kinetics of gas phase reactions, kinetics of decomposition of N_2O_5, H_2-Cl_2 photochemical reaction and H_2-Br_2 thermal reaction; explosion limits, oscillatory reactions, Lotka-Voltra mechanism, autocatalysis, chemical chaos. Michaelis-Menten enzyme kinetics; temperature, pH and concentration dependence of enzyme catalyzed reactions.	12
II	**Reaction Dynamics** Collisions of real molecules, theories of reaction rates: Arrhenius theory; collision theory, activated complex theory, Kramer's theory, Lindeman's theory of uni-molecular reactions. Experimental methods for studying fast reactions, flash photolysis, shock tube, molecular beam and relaxation techniques, dynamics of molecular collisions and potential energy	18

	surfaces. Reactions in solutions: Factors determining reaction rates in solution, reactions involving ion-ion and ion-dipoles reaction; influence of solvent, ionic strength and pressure on the reactions in solution. Kinetics of photochemical and photophysical process, quantum yield, quenching, excited states, energy transfer processes, Marcus theory of electron transfer process	
III	**Molecular Dynamics** Concept of molecular dynamics: Phase space, number of states, density of states. Force field: bonded and non bonded interactions, MM and QM force field. Equation of motion. Trajectory calculation. Concept of multi scale modeling	06

Essential Readings:

1. K. J. Laidler, “Chemical Kinetics”, Prentice Hall, 3rd Edition, 2003.

Supplementary Readings:

1. P. Atkins and J. D. Paula, “Atkins' Physical Chemistry”, Oxford University Press, 10th Edition 2014
2. J. I. Steinfeld, J. S. Francisco, W. L. Hase, “Chemical Kinetics and Dynamics”, Pearson, 2nd Edition, 1998.
3. S. K. Upadhyay, “Chemical Kinetics and Reaction Dynamics” Springer, 2006 Edition