Semester	JAN 2022
Open to semester	14,22
Course code	**CH6432**
Course title	**Introduction to Machine Learning in Chemistry**
Credits	2 /2
Course Coordinator & participating faculty (if any)	Arnab Mukherjee
Nature of Course	Lectures
Pre-requisites	Knowledge of basic programming in any language (say, python) and basic mathematical skills (Linear algebra, basic statistics and probability concepts)
Objectives (goals, type of students for whom useful, outcome etc)	Machine learning and deep learning are new tools of research applied to practically every scientific field. Chemistry is also not an exception. While the basics of machine learning is common to each area, this course will highlight the possibility of applications of this topic in chemistry. After covering the basics of machine learning and deep learning, the course will take examples from various published article to understand where and how it is applied. Since this course is meant for the Ph.D. students, the goal is to show the usage of machine learning in the research areas of chemistry.
Course contents (details of topics /sections with no. of lectures for each)	• Introduction: How do machines learn and what to learn in chemistry • Prerequisite Revision: Review of Basic mathematical and programming tools • Various topics of ML in Chemistry: drug design, material design etc.
Evaluation /assessment	End-Sem Examination-% Mid-Sem Examination-% Others-The evaluation will be based on completion of a project from any research paper or a given topic (reproducing the results of a research paper). The marks will depend on the level of difficult and clarity of understanding during the presentation of the work. %
Suggested readings (with full list of authors, publisher, year, edn etc.)	1. Machine Learning in Chemistry: The impact of Artificial Intelligence, Ed. Hugh M. Cartwright, RSC, UK (2020) 2. Research publications on the topic