CHEM6134: AI FOR CHEMISTRY

Effective Term
Semester A 2026/27

Part I Course Overview

Course Title
AI for Chemistry

Subject Code
CHEM - Chemistry
Course Number
6134

Academic Unit
Chemistry (CHEM)

College/School
College of Science (SI)

Course Duration
One Semester

Credit Units
3

Level
P5, P6 - Postgraduate Degree

Medium of Instruction
English

Medium of Assessment
English

Prerequisites
Nil

Precursors
Nil

Equivalent Courses
Nil

Exclusive Courses
Nil

Additional Information
Nil

Part II Course Details

Abstract

The proposed AI for Chemistry course is designed to enable postgraduate students to deeply understand the integration of artificial intelligence technologies with chemical research and applications. The course covers fundamental concepts and working principles of AI methods such as machine learning, deep learning, and neural networks, and their applications in diverse chemical disciplines, including drug discovery, materials science, computational chemistry, and analytical sciences. Through critical review and discussion of recent literature, students will explore the latest AI-driven advancements in areas like molecular modeling, reaction prediction, and spectroscopic analysis, evaluating their advantages, limitations, and challenges for chemical R&D. Individual literature reviews will prompt students to identify current chemical problems and propose innovative AI-based approaches to derive chemical insights. Upon completion, students will be capable of designing AI-empowered experimental strategies or computational workflows, combining appropriate AI tools to address complex problems in chemistry.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Explain and apply fundamental AI concepts and algorithms (e.g., machine learning, deep learning, neural networks) in chemical research, including their principles in molecular modeling, property prediction, and reaction dynamics simulation.	30	x	x	
2	Discuss the latest AI-driven advancements in chemistry (e.g., AI-based drug design, materials discovery, spectroscopic analysis), and critically evaluate their advantages, limitations, and ethical challenges in research and industry.	40	x	x	
3	Propose innovative AI solutions for modern chemical problems (e.g., data-driven synthesis planning, automated experimental design), and justify the selection of appropriate AI methods or their integration with traditional chemical techniques.	30	x	x	x

A1: Attitude
Develop an attitude of discovery/innovation/creativity, as demonstrated by students possessing a strong sense of curiosity, asking questions actively, challenging assumptions or engaging in inquiry together with teachers.

A2: Ability
Develop the ability/skill needed to discover/innovate/create, as demonstrated by students possessing critical thinking skills to assess ideas, acquiring research skills, synthesizing knowledge across disciplines or applying academic knowledge to real-life problems.

A3: Accomplishments
Demonstrate accomplishment of discovery/innovation/creativity through producing /constructing creative works/new artefacts, effective solutions to real-life problems or new processes.

Learning and Teaching Activities (LTAs)

	LTAs	Brief Description	CILO No.	Hours/week (if applicable)
1	Lectures	Student will learn core AI concepts (machine learning, deep learning) and their applications in chemistry, such as molecular property prediction and reaction modeling. Through problem-solving sessions, students will apply AI algorithms to analyze chemical data, reinforcing understanding of fundamental principles.	1, 2, 3	26 hours in total
2	Assignments	Students will analyze recent research papers on AI-driven innovations in chemistry (e.g., AI-based drug design, materials discovery) based on selected topics. Students will perform evaluations of technical approaches, validate results, and critique the advantages and limitations of AI methods in real-world chemical research.	1, 2	6 hours in total
3	Group Projects & Presentation	Students will collaborate to design AI solutions for chemical challenges (e.g., developing models to predict catalyst efficiency or optimize synthesis conditions). Using the fundamental AI-related tools, the students will implement, validate, and present AI models, justifying method selection and evaluating impact on problem-solving.	3	7 hours in total

Assessment Tasks / Activities (ATs)

	ATs	CILO No.	Weighting (%)	Remarks ("-" for nil entry)	Allow Use of GenAI?
1	AI Principles & Chemical Applications Assignment Evaluate understanding of AI fundamentals (machine learning, deep learning, neural networks) and their applications in chemistry.	1, 2	30	-	Yes
2	AI Model Design Project and Presentation Design a hypothetical AI model (e.g., a hybrid machine learning approach) to solve a specific chemical problem (e.g., predicting protein-ligand binding affinity).	3	30	-	Yes

Continuous Assessment (%)

60

Examination (%)

40

Examination Duration (Hours)

2

Minimum Continuous Assessment Passing Requirement (%)

40

Minimum Examination Passing Requirement (%)

40

Assessment Rubrics (AR)

Assessment Task

AI Principles & Chemical Applications Assignment

Criterion

Accurately explain AI principles (e.g., machine learning, graph neural networks) and their adaptation to chemical contexts; Scientifically justify the application of AI techniques to solve chemical problems (e.g., property prediction, reaction design); Critically analyze AI’ s advantages, limitations, and innovative potential in chemical research.

Excellent

(A+, A, A-) High
Explains AI principles with few errors; proposes scientifically rigorous AI applications tightly linked to chemical contexts; deeply analyzes AI limitations and proposes innovative solutions.

Good

(B+, B, B-) Significant
Explains AI principles with some errors; proposes reasonable AI applications aligned with chemical problems; identifies common AI limitations and suggests standard solutions.

Fair

(C+, C, C-) Basic
Demonstrates basic understanding of AI principles with partial technical errors; AI applications have general relevance to chemical problems but lack depth.

Marginal

(D) Minimal
Partially understands AI principles; AI applications are disconnected from chemical contexts; lacks meaningful analysis of AI limitations.

Failure

(F) Not even reaching marginal levels
Fails to grasp core AI principles; AI applications contain scientific errors; does not meet assignment requirements.

Assessment Task

AI Model Design Project and Presentation

Criterion

1. Technical Design: Rationality of AI model architecture, data processing logic, and accuracy of algorithm adaptation to chemical problems.
2. Chemical Relevance: Focus on solving real-world chemical issues (e.g., molecular design, reaction prediction) and alignment with chemical theory.
3. Innovation: Novelty of model design, improvements over existing methods, and analysis of limitations with proposed solutions.
4. Presentation Effectiveness: Clarity of structure, effectiveness of visual materials, fluency of oral delivery, and responsiveness in Q&A.

Excellent

(A+, A, A-) High
Rigorous and innovative model design, precisely addressing significant chemical problems; clear presentation with in-depth limitation analysis and optimization proposals.

Good

(B+, B, B-) Significant
Reasonable model design solving relevant chemical problems; structured presentation with analysis of common limitations and solutions.

Fair

(C+, C, C-) Significant

Basically feasible model design with general chemical relevance; relatively clear presentation with superficial limitation analysis.

Marginal

(D) Minimal
Obvious flaws in model design, weak chemical relevance; disorganized presentation with insufficient analysis.

Failure

(F) Not even reaching marginal levels
Scientifically flawed model design, irrelevant to chemical problems; incomplete or severely missing presentation content.

Assessment Task

Examination

Criterion

Ability to explain in detail and with accuracy the principles of advanced AI techniques, discuss and critically evaluate their advantages, limitations, and challenges, propose and justify their applications for modern chemical research.

Excellent

(A+, A, A-) High
Able to correctly answer almost all the examination questions precisely and concisely with no errors

Good

(B+, B, B-) Significant
Able to correctly answer a substantial number of the examination questions precisely and concisely with no errors

Fair

(C+, C, C-) Basic
Able to correctly answer most of the examination questions precisely and concisely with only a few errors

Marginal

(D) Minimal
Able to present a few required knowledge and concepts with some errors; and able to propose reasonable instrumental approaches with scientific basis

Failure

(F) Not even reaching marginal levels
Unable to correctly answer most of the examination questions

Part III Other Information

Keyword Syllabus

Artificial intelligence; Machine learning; Deep learning; Neural networks; Graph neural networks; Transformer models; Reinforcement learning; Molecular dynamics; Drug discovery; Catalyst design; Materials informatics; Reaction prediction; Retrosynthesis; Property prediction; TensorFlow; DeepChem; Physics-informed AI; Quantum machine learning; Explainable AI; Data scarcity; Ethical AI; Synthetic chemistry automation; High-throughput screening; AI-driven spectroscopy; Multiscale modeling; AI-robotics integration; Sustainable chemistry

Reading List

Compulsory Readings

	Title
1	Nil

Additional Readings

	Title
1	Machine Learning in Chemistry; Jon Paul Janet, Heather J. Kulik (American Chemical Society, 2020)
2	AI and Robotic Technology in Materials and Chemistry Research; Xi Zhu (Wiley, 2024)
3	Applications of Artificial Intelligence in Chemistry; Hugh M. Cartwright (Oxford University Press, 1994)