MSE6183: COMPUTATIONAL METHODS FOR MATERIALS SCIENCE

Effective Term
Semester A 2025/26

Part I Course Overview

Course Title
Computational Methods for Materials Science

Subject Code
MSE - Materials Science and Engineering

Course Number
6183

Academic Unit
Materials Science and Engineering (MSE)

College/School
College of Engineering (EG)

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
AP6172 Simulation and Modelling in Multidisciplinary Sciences (From the old curriculum)

Exclusive Courses
Nil

Part II Course Details

Abstract

Basic concepts of computer modeling in science and engineering using discrete particle systems and continuum fields. Techniques and software for statistical sampling, simulation, data analysis and visualization. Use of statistical, molecular dynamics, Monte Carlo, mesoscale and continuum methods to study fundamental physical phenomena encountered in the fields of computational materials science, physics, and chemistry. Applications drawn from a range of disciplines to build a broad-based understanding of complex structures and interactions in problems where simulation is on equal-footing with theory and experiment. Term project allows development of individual interest.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Student will identify the importance of simulation and modeling in materials science.	10	x		
2	Demonstrate a few problems in materials science using simulation and modelling tools.	20		x	
3	Identify the key variables that determine the quality and reliability of simulation and modelling.	15	x		
4	Identify state-of-the-art developments in the relevant area, to form opinions on specific issues and to demonstrate independent problem-solving ability.	15			x
5	Apply basic simulation and modelling tools to solve simple problems in one of the following areas: materials science, physics, chemistry, and life science.	40	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	1	Lectures	1, 2, 3, 4	20hrs/10wks (wk: 1-8,10-11)
2	2	Tutorials	1, 2, 3, 4	5hrs/5wks (wk: 2,4,6,8,11)
3	3	Project	5	16hrs/4wks (last 4 wks)

Assessment Tasks / Activities (ATs)

	ATs	CILO No.	Weighting (%)	Remarks ("-" for nil entry)	Allow Use of GenAI?
1	Assignments	1, 2, 3, 4	20	performance assessment purpose	Yes
2	Project	5	40	Inc. project report and presentation	Yes
3	Mid-term Test	1, 2, 3, 4	40	-	No

Continuous Assessment (%)

100

Assessment Rubrics (AR)

Assessment Task

Assignments (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure

(F) Not reaching marginal level

Assessment Task

Mid-term Test (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion

He/she can thoroughly identify and explain how the principles are applied to science and technology for solving materials science problems.

Excellent

(A+, A, A-) High

Good

(B+, B, B-) Significant

Fair

(C+, C, C-) Moderate

Marginal

(D) Basic

Failure
(F) Not reaching marginal level

Assessment Task
Project (for students admitted before Semester A 2022/23 and in Semester A 2024/25 & thereafter)

Criterion
The student's may formulate a simulation method using the course materials, solve a scientific problem, explain the results and conclusions, and present in class. He/she is able to communicate ideas effectively and persuasively via written texts and/or oral presentation.

Excellent
(A+, A, A-) High

Good
(B+, B, B-) Significant

Fair
(C+, C, C-) Moderate

Marginal
(D) Basic

Failure
(F) Not reaching marginal level

Assessment Task
Assignments (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion
The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.

Excellent
(A+, A, A-) High

Good
(B+, B) Moderate

Marginal
(B-, C+, C) Basic

Failure
(F) Not reaching marginal level

Assessment Task
Mid-term Test (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

He/she can thoroughly identify and explain how the principles are applied to science and technology for solving materials science problems.

Excellent

(A+, A, A-) High

Good

(B+, B) Moderate

Marginal

(B-, C+, C) Basic

Failure

(F) Not reaching marginal level

Assessment Task

Project (for students admitted from Semester A 2022/23 to Summer Term 2024)

Criterion

The student's may formulate a simulation method using the course materials, solve a scientific problem, explain the results and conclusions, and present in class. He/she is able to communicate ideas effectively and persuasively via written texts and/or oral presentation.

Excellent

(A+, A, A-) High

Good

(B+, B) Moderate

Marginal

(B-, C+, C) Basic

Failure

(F) Not reaching marginal level

Part III Other Information

Keyword Syllabus

- Introduction
Advances in computational methods and tools. Computer-aided design and simulation in multidisciplinary areas including materials science, physics, chemistry, and life science.
- Monte Carlo methods
History. Applications areas. Use in mathematics. Monte Carlo and random numbers.
- Molecular dynamics simulation
Areas of Application. Design Constraints. Potentials. Molecular dynamics algorithms.
- Continuum Methods
Conservation Laws, continuum equations, finite difference method for phase transition, dendritic solidification, thermal transport
- Numerical optimization methods
Conjugate gradient method. Simulated annealing. Genetic algorithms.
- Project

A discovery oriented multidisciplinary project such as new materials design, new physics exploration, or drug design.

Reading List

Compulsory Readings

	Title
1	"Monte Carlo method", http://en.wikipedia.org/wiki/Monte_Carlo_method
2	"Molecular dynamics", http://en.wikipedia.org/wiki/Molecular_dynamics
3	"Mathematical optimization", http://en.wikipedia.org/wiki/Mathematical_optimization

Additional Readings

	Title
1	K Binder, D W Heermann, "Monte Carlo Simulation in Statistical Physics: An Introduction", Berlin : Springer-Verlag, 1988. (C0092255)
2	Daan Frenkel, Berend Smit, "Understanding Molecular Simulation: From Algorithms to Applications", San Diego: Academic Press, 1996. (QD461 .F86 1996)
3	Alexander K Hartmann, Heiko Rieger, "Optimization Algorithms in Physics", Berlin: Wiley-VCH, 2002. (QC20.7.C58 H37 2002)
4	David P Landau, Kurt Binder, "A Guide to Monte Carlo Simulations in Statistical Physics", Cambridge, UK; New York: Cambridge University Press, 2005. (QC174.85.M64 L36 2005)
5	Kurt Binder, "Monte Carlo and Molecular Dynamics Simulations in Polymer Science [electronic resource]", New York: Oxford University Press, 1995. (QD381.9.E4 M66 1995eb)