MSE4119: MODELING MATERIALS: A COURSE POWERED BY AI

Effective Term
Semester A 2025/26

Part I Course Overview

Course Title
Modeling Materials: a Course Powered by AI

Subject Code
MSE - Materials Science and Engineering

Course Number
4119

Academic Unit
Materials Science and Engineering (MSE)

College/School
College of Engineering (EG)

Course Duration
One Semester

Credit Units
3

Level
B1, B2, B3, B4 - Bachelor's Degree

Medium of Instruction
English

Medium of Assessment
English

Prerequisites
MSE3114 Fundamentals of Scientific Computing: a Course Powered by AI

Precursors
Nil

Equivalent Courses
Nil

Exclusive Courses
MSE6183 Computational Methods for Materials Science

Part II Course Details

Abstract

This class will introduce concepts of computer modeling and simulation in materials science and engineering using both discrete particle (atomic, molecular) systems and continuum fields. Apply statistical mechanics, molecular dynamics, Monte Carlo, mesoscale and continuum methods to study fundamental physical phenomena encountered in the fields of computational materials science, physics, and chemistry. Techniques for statistical sampling, simulation, data analysis and visualization. Applications drawn from a wide 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. An individual project or term project allows the development of individual interest.

Course Intended Learning Outcomes (CILOs)

	CILOs	Weighting (if app.)	DEC-A1	DEC-A2	DEC-A3
1	Identify the importance of simulation and modeling in materials science.	20	x		
2	Identify the key variables that determine the quality and reliability of simulation and modeling.	20	x		
3	Apply the basic concepts, theories and tools to a discovery oriented project in student' s own discipline such as: new materials design, new physics exploration, drug design, etc.	40			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.	20			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	Students will engage in formal lectures to gain knowledge about different modeling and simulation methods for materials science.	1, 2, 3, 4	3hrs/wk
2	Tutorials	Students will engage in tutorial activities to operate modeling software, run simulation, data analysis and visualization.	1, 2, 4	1hr/wk

3	Projects	Students will participate in groups to consolidate their learning as they produce reports integrating the knowledge learned in lectures, tutorials and their own, and will actively engage as audience members during peers' presentations in order to expand their own knowledge	3	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, 4	20	performance assessment purpose	No
2	Project	3	40	Inc. project report and presentation	No
3	Mid-term Test	1, 2, 3, 4	40	-	No

Continuous Assessment (%)

100

Examination (%)

0

Assessment Rubrics (AR)

Assessment Task

1. Assignments

Criterion

Students can complete 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
2. Mid-term Test

Criterion
Students 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
3. Project

Criterion
The student's work shows strong evidence of original thinking, supported by a variety of properly documented information sources other than taught materials. Students are 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

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.

- Molecular dynamics simulation

Areas of Application. Design Constraints. Potentials. Molecular dynamics algorithms.

- Continuum Methods

Conservation Laws, order parameter, phase field theory, continuum equations, finite difference method for phase transition, dendritic solidification, thermal transport

- Monte Carlo methods

History. Applications areas. Monte Carlo and random numbers.

- Numerical optimization methods

Conjugate gradient method. Simulated annealing.

- Project

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

Reading List

Compulsory Readings

	Title
1	“Understanding Molecular Simulation: From Algorithms to Applications”, San Diego: Academic Press, 1996.
2	Nikolas Provatas and Ken Elder, Phase-Field Methods in Materials Science and Engineering, 2011
3	Christophe Chipot, Numerical Methods for molecular Dynamics Simulations of Biological Systems, 2010

Additional Readings

	Title
1	K Binder, D W Heermann, “Monte Carlo Simulation in Statistical Physics: An Introduction”, Berlin : Springer-Verlag, 1988. (C0092255)
2	“Monte Carlo method”, http://en.wikipedia.org/wiki/Monte_Carlo_method
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)
6	“Mathematical optimization”, http://en.wikipedia.org/wiki/Mathematical_optimization
7	“Molecular dynamics”, http://en.wikipedia.org/wiki/Molecular_dynamics