City University of Hong Kong
Course Syllabus

offered by Department of Materials Science and Engineering
with effect from Semester A 2022/23

Part I Course Overview

Course Title:	**Computational Methods for Materials Science**
Course Code:	**MSE6183**
Course Duration:	**One semester**
Credit Units:	**3**
Level:	**P6**
Medium of Instruction:	**English**
Medium of Assessment:	**English**
Prerequisites: *(Course Code and Title)*	**Nil**
Precursors: *(Course Code and Title)*	**Nil**
Equivalent Courses: *(Course Code and Title)*	**AP6172 Simulation and Modelling in Multidisciplinary Sciences (From the old curriculum)**
Exclusive Courses: *(Course Code and Title)*	**Nil**

Part II Course Details

1. Abstract

(A 150-word description about the course)

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.

2. Course Intended Learning Outcomes (CILOs)

(CILOs state what the student is expected to be able to do at the end of the course according to a given standard of performance.)

No.	CILOs	Weighting* (if applicable)	Discovery-enriched curriculum related learning outcomes (please tick where appropriate)		
			A1	*A2*	*A3*
1.	Recognize the importance of simulation and modeling in materials science.	10%	√		
2.	Demonstrate a few problems in materials science using simulation and modelling tools.	20%		√	
3.	Identify the key variables that determine the quality and reliability of simulation and modelling.	10%	√		
4.	Apply basic simulation and modelling tools to solve simple problems in one of the following areas: materials science, physics, chemistry, and life science.	25%			√
5	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.	25%			√
6	Identify state-of-the-art developments in the relevant area, to form opinions on specific issues and to demonstrate independent problem-solving ability.	10%	√		
	** If weighting is assigned to CILOs, they should add up to 100%.*	100%			

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 self-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.

3. Teaching and Learning Activities (TLAs)

(TLAs designed to facilitate students' achievement of the CILOs.)

TLA	Brief Description	CILO No.						Hours/week (if applicable)
		1	**2**	**3**	**4**	**5**	**6**	
1	Lectures	√	√	√	√			20hrs/10wks (wk: 1-8,10-11)
2	Tutorials	√	√	√	√			5hrs/5wks (wk: 2,4,6,8,11)
3	Project					√	√	16hrs/4wks (last 4 wks)

4. Assessment Tasks/Activities (ATs)

(ATs are designed to assess how well the students achieve the CILOs.)

Assessment Tasks/Activities	CILO No.						Weighting*	Remarks
	1	2	3	4	5	6		
Continuous Assessment: 100%								
Assignments	√	√	√	√			20%	performance assessment purpose
Project					√	√	40%	Inc. project report and presentation
Mid-term Test	√	√	√	√			40%	
Examination: 0%								
** The weightings should add up to 100%.*							100%	

5. Assessment Rubrics

(Grading of student achievements is based on student performance in assessment tasks/activities with the following rubrics.)

Applicable to students admitted in Semester A 2022/23 and thereafter

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B)	Marginal (B-, C+, C)	Failure (F)
1. Assignments	The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.	High	Moderate	Basic	Not reaching marginal level
2. Mid-term Test	He/she can thoroughly identify and explain how the principles are applied to science and technology for solving materials science problems.	High	Moderate	Basic	Not reaching marginal level
3. Project	The student's work shows strong evidence of original thinking, supported by a variety of properly documented information sources other than taught materials. He/she is able to communicate ideas effectively and persuasively via written texts and/or oral presentation.	High	Moderate	Basic	Not reaching marginal level

Applicable to students admitted before Semester A 2022/23

Assessment Task	Criterion	Excellent (A+, A, A-)	Good (B+, B, B-)	Fair (C+, C, C-)	Marginal (D)	Failure (F)
1. Assignments	The student completes all assessment tasks/activities and the work demonstrates excellent understanding of the scientific principles and the working mechanisms.	High	Significant	Moderate	Basic	Not reaching marginal level
2. Mid-term Test	He/she can thoroughly identify and explain how the principles are applied to science and technology for solving materials science problems.	High	Significant	Moderate	Basic	Not reaching marginal level
3. Project	The student's work shows strong evidence of original thinking, supported by a variety of properly documented information sources other than taught materials. He/she is able to communicate ideas effectively and persuasively via written texts and/or oral presentation.	High	Significant	Moderate	Basic	Not reaching marginal level

Part III Other Information (more details can be provided separately in the teaching plan)

1. Keyword Syllabus

(An indication of the key topics of the course.)

- 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
- Ab-Initio Calculations (optional)
  First-principles quantum mechanics and density functional theory (DFT) calculations
- 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.

2. Reading List

2.1 Compulsory Readings

(Compulsory readings can include books, book chapters, or journal/magazine articles. There are also collections of e-books, e-journals available from the CityU Library.)

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

2.2 Additional Readings

(Additional references for students to learn to expand their knowledge about the subject.)

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)