Course guide
295910 - SAMEB - Advanced Simulation of Materials for Engineering and Bioengineering

Last modified: 19/06/2026

Unit in charge: Barcelona East School of Engineering
Teaching unit: 713 - EQ - Department of Chemical Engineering.

Degree: BACHELOR'S DEGREE IN BIOMEDICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Optional subject).
BACHELOR'S DEGREE IN MATERIALS ENGINEERING (Syllabus 2010). (Optional subject).

Academic year: 2026 **ECTS Credits:** 6.0 **Languages:** English

LECTURER

Coordinating lecturer: Juan Torras Costa

Others: David Zanuy Gomara
Juan Torras Costa

PRIOR SKILLS

Basic knowledge of chemistry and physics

TEACHING METHODOLOGY

The course consists of four hours a week in the computer lab: two correspond to lectures and guided practical exercises in a computer. The other two class hours will be devoted to the development of a computer simulation project.
The syllabus will be divided into four parts and in each one the student will have to carry out an out-of-class work based on the simulation projects developed in the computer lab. Throughout the course, different scientific papers on the computational simulation field will be studied in groups to be exposed and discussed in class later.

LEARNING OBJECTIVES OF THE SUBJECT

A subject based on short-term projects and objectives will be raised. The student will make a set of practical examples of atomistic simulations of advanced materials that will be developed throughout the course to understand their behavior, the interrelation with their environment, and focused on the field of Chemical Engineering, materials , of catalysis and bioengineering. Through computational simulation techniques, the student is expected to have a more explicit vision of the different levels of organization of matter depending on the scale and the time frame of the physical phenomena they study at the experimental level.

The main training objectives are:
• Familiarize students with the basic concepts of atomistic simulation of materials and biomaterials
• Provide tools for the visualization and manipulation of atomistic systems for engineering and bioengineering
• Familiarize students in simulation techniques based on molecular dynamics

STUDY LOAD

Type	Hours	Percentage
Self study	90,0	60.00
Hours small group	15,0	10.00
Hours large group	45,0	30.00

Total learning time: 150 h

CONTENTS

1. Introduction to molecular modeling

Description:
• Introduction
• The working environment: Linux operating system
• Basic Linux commands
• Scripts
• Description and representation of atomistic models

Related activities:
• Theory classes and guided exercises
• Practice 1: Introduction to Linux

Full-or-part-time: 30h
Theory classes: 4h
Practical classes: 8h
Self study : 18h

2. Classic model. Conformational studies of materials and proteins

Description:
• Representation and visualization of crystals, amorphous materials and proteins
• Representation of atomic interactions: force-field
• Molecular dynamics of systems

Related activities:
• Theoretical classes and guided exercises
• Practice 2: Structural study of a polymer, crystal and/or protein

Full-or-part-time: 30h
Theory classes: 4h
Practical classes: 8h
Self study : 18h

3. Quantum model. Heterogeneous and enzymatic catalysis

Description:
• Modeling of systems involving chemical reactions
• Quantum simulation techniques

Related activities:
• Theoretical classes and guided exercises
• Practice 3: Simulation of a heterogeneous and/or enzymatic catalysis process

Full-or-part-time: 30h
Theory classes: 4h
Practical classes: 8h
Self study : 18h

4. Applications. Advanced simulation of materials

Description:
• Polymers
• Hybrid materials and heterogeneous systems
• Enzymatic processes
• Structural bioinformatics: Fast threading, homology, computer drug design

Related activities:
• Theoretical classes and guided exercises
• Practice 4: Open simulation practice (to be chosen from a finite set)

Full-or-part-time: 60h
Theory classes: 8h
Practical classes: 16h
Self study : 36h

GRADING SYSTEM

Any academic fraud, plagiarism or use or possession of unauthorised means in an assessment activity leads to a mark of zero (0) for the affected test or assignment. Furthermore, in accordance with the University's regulations, if disciplinary proceedings are initiated the subject is recorded as "Pending Assessment" until a decision is reached. These incidents are managed in accordance with the **Action Framework for Academic Integrity in Assessment at the UPC**.

The evaluation of the subject will be carried out through the assessment of each of the four projects that are developed throughout the course (4 x 20% = 80%) and the exhibition work in class about the studied scientific paper (20%).

EXAMINATION RULES.

No final test

BIBLIOGRAPHY

Basic:
- Leach, Andrew R. Molecular modelling : principles and applications. 2nd ed. Harlow [etc.]: Addison Wesley, 2001. ISBN 0582382106.

Complementary:
- Cramer, Christopher J.. Essentials of computational chemistry : theories and models. 2nd ed. Wiley John & Sons, 2004. ISBN 9780470091821.
- van Santen, Rutger A.. Modern heterogeneous catalysis : an introduction. Wiley-VCH Verlag GmbH & Co. KGaA, 2017. ISBN 9783527339617.