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

**Last modified:** 27/05/2024

**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:** 2024 **ECTS Credits:** 6.0 **Languages:** Catalan, Spanish, English

## LECTURER

**Coordinating lecturer:** Joan Torras Costa

**Others:** Segon quadrimestre:
JOAN TORRAS COSTA - M10
DAVID ZANUY GOMARA - M10
DAVID NARANJO TOVAR - M10

## 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

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.