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

Coordinating unit: 295 - EEBE - Barcelona East School of Engineering
Teaching unit: 713 - EQ - Department of Chemical Engineering
Academic year: 2019
Degree: BACHELOR’S DEGREE IN BIOMEDICAL ENGINEERING (Syllabus 2009). (Teaching unit Optional)
BACHELOR’S DEGREE IN CHEMICAL ENGINEERING (Syllabus 2009). (Teaching unit Optional)
BACHELOR’S DEGREE IN MATERIALS ENGINEERING (Syllabus 2010). (Teaching unit Optional)
ECTS credits: 6 Teaching languages: Catalan, Spanish, English

Teaching staff
Coordinator: Juan Torras Costa
Others: David Zanuy Gomara
Guillem Revilla López
Didac Martí Ballesté

Opening hours
Timetable: To be announced at the beginning of the semester.

Prior skills
Basic knowledge of chemistry and physics

Requirements
Have surpassed the subjects that provide the previous indicated capacities of the initial phase.

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

## Content

<table>
<thead>
<tr>
<th>Section</th>
<th>Learning time: 30h</th>
</tr>
</thead>
</table>

| | Theory classes: 4h |
| | Practical classes: 8h |
| | Self study: 18h |

### 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

### 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

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

4. Applications. Advanced simulation of materials

<table>
<thead>
<tr>
<th>Learning time: 60h</th>
</tr>
</thead>
<tbody>
<tr>
<td>Theory classes: 8h</td>
</tr>
<tr>
<td>Practical classes: 16h</td>
</tr>
<tr>
<td>Self study: 36h</td>
</tr>
</tbody>
</table>

**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)

**Qualification 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%).

**Regulations for carrying out activities**

No final test

**Bibliography**

**Basic:**


**Complementary:**
