27230 - Introduction to Molecular Modeling

Syllabus Information

Academic year: 2024/25
Subject: 27230 - Introduction to Molecular Modeling
Faculty / School: 100 - Facultad de Ciencias
Degree: 452 - Degree in Chemistry
ECTS: 5.0
Year: 4
Semester: Second semester
Subject type: Optional
Module:

1. General information

The subject has the following approaches and objectives:

- Introduce students to the basic aspects of the methods and techniques used to computationally model chemical systems at a molecular scale.
- Use computer programs to model and obtain information for a wide range of chemical problems such as molecular structure, molecular properties, chemical reactivity or chemical bonding, among others.
- Understand issues of a chemical nature at the molecular level.

It is an optional subject of the advanced module of the Chemistry degree (corresponding to the 4th year). It is taught in the second semester and it is recommended to have taken Physical Chemistry II

The subject serves to acquire knowledge and skills in the field of molecular modeling, emphasizing the practical use of computational chemistry software.

2. Learning results

- Know the concepts and basic aspects of molecular modeling, as well as the use of computer programs.
- Select the level of calculation most appropriate to the experimental problem.
- Carry out computational modeling of simple chemical reactions and properties of the electronic structure at a molecular scale.
- Propose, locate and characterize stable molecular structures, obtaining their chemical and physical properties.
- Know how to carry out the theoretical calculation of kinetic and thermodynamic parameters of simple organic reactions.
- Analyze basic biochemical systems.
- Prepare and present reports of results or studies carried out by him or herself or by others.

The importance of these results lies in the fact that computational chemistry is a tool used by many areas of chemistry to understand and predict structures, reactivity or properties of molecules or chemical systems in general.

3. Syllabus

1. Theory: Methods of Computational Chemistry

Introduction to Computational Chemistry.

Molecular Mechanics Methods or Force Fields (MM).

Quantum chemical methods or electronic structure methods (QM).

Hartree-Fock and electronic correlation method. Introduction to density functional theory (DFT).

Bonding, structure and chemical reactivity.

Introduction to molecular calculation and visualization programs. Web resources.

2. Application of molecular calculation programs to various chemical problems:

Potential energy hypersurfaces, geometry optimization, energy obtaining.

Determination of molecular and spectroscopic properties.

Solvent effect and non-covalent interactions.

Organic reactivity, kinetic isotopic effect.

Homogeneous organometallic catalysis.

Conformational analysis and dynamics of proteins.

4. Academic activities

Activity 1: Acquisition of theoretical content (2.5 ECTS) in participatory group master classes.

Activity 2: Computer practices carried out individually and supervised by the teacher in the use of computational chemistry computer programs (0.3 ECTS).

Activity 3: Practices in a computer laboratory on molecular modeling problems (2.2 ECTS).

Attendance at practices, completion and presentation of the requested reports are mandatory.

5. Assessment system

The evaluation activities are the following:

1. The work carried out in the computer classroom practices and delivery of results reports. A total of 4 practice reports will be delivered. A template will be available to prepare each report. This block represents 50 % of the final grade.
2. Written evaluation test (maximum duration of 1 hour) of the theoretical contents: 25 % of the final grade.
3. Autonomous team work (2-3 students). A joint report will be presented (maximum 10 pages) whose grade will account for 25 % of the final grade.

Students who have not completed all the practices and activities will be evaluated through a global test on the two official calls.

6. Sustainable Development Goals

4 - Quality Education
7 - Affordable and Clean Energy
9 - Industry, Innovation and Infrastructure