Universidad Zaragoza

Academic Year/course: 2023/24

60457 - Molecular modelling

Syllabus Information

Academic year: 2023/24
Subject: 60457 - Molecular modelling
Faculty / School: 100 - Facultad de Ciencias
Degree: 543 - Master's in Molecular Chemistry and Homogeneous Catalysis
ECTS: 2.0
Year: 1
Semester: Second semester
Subject type: Optional
Module:

1. General information

The subject aims to introduce the student to the methods of computational chemistry since computational results are an increasingly common part of the results presented in the primary literature in chemistry. To this end, the student will be introduced to the theoretical basis necessary to, at least, critically understand the results presented.

An important part of it is the understanding of the methodology of computational studies. For this purpose, a simple practical application will be performed.

These approaches and objectives are aligned with the following Sustainable Development Goals (SDGs) of the United Nations Agenda 2030 (https://www.un.org/sustainabledevelopment/en/), such that the acquisition of the learning results of the subject provides training and competence to contribute to some extent to their achievement, particularly in relation to goals: 4, quality education; 7, affordable and clean energy; and 12, responsible production and consumption.

2. Learning results

To understand the computational chemistry methods used in the study of organic or inorganic molecules and be able to use them appropriately for the study of molecular structure, spectroscopic properties and chemical reactivity, including reaction mechanisms.
To understand the theoretical component of a combined experimental/computational study and assess the relevance of the theoretical input.
To understand the concept of potential energy surface, how it is explored and represented, and its relationship to the mechanism of a reaction.
To understand how molecular orbitals, electron population analyses, electron densities or molecular electrostatic potentials can be used in the interpretation of chemical bonding and reactivity.
To understand the role of solvent and solvation in chemical reactivity and how it can be treated from a theoretical point of view.
To apply the concepts derived from computational chemistry to the analysis and solving of chemical problems, as well as to the understanding of the synthesis, structure and reactivity of chemical compounds.

3. Syllabus

The program of the subject consists of the following topics:
1.- Introduction to computational chemistry.
2.- Introduction to the use of computational environments and application programs in chemistry.
3.- Concept of potential surface.
4.- Theoretical quantum chemical methods WFT and DFT.
5.- Applications to the study of molecular structure, reactivity and reaction mechanisms.
6.- Use of computational chemistry programs.

4. Academic activities

Expository-participative classes (1.2 ECTS).
Problem solving and seminars (0.2 ECTS).
Computer practice (0.6 ECTS)
Small group or personalized tutoring.

5. Assessment system

The continuous assessment of this subject is based on a practical test to be carried out in the global assessment period

consisting of the solving of problems and theoretical-practical questions similar to those dealt with in the subject (100%).

The final grade will be that of the global test

The number of official exams to which the enrolment entitles the student (2 per enrolment) as well as the use of these calls for exams will be in accordance with the *Rules of Permanence in Master's Studies* and the *Rules for the Evaluation of Learning* (https://ciencias.unizar.es/normativas-asuntos-academicos) In accordance with the same, the time, place and date of the review will be made public when the grades are published.