60457 - Molecular modelling

Información del Plan Docente

Academic Year	2017/18
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

1.1.Introduction

This subject tries to initiate the students to the methods of computational chemistry in order to make them able, at least, to understand in a critical way the results which are presented in primary bibliography related to their work area.

1.2.Recommendations to take this course

Previous background on Quantum Chemistry (at the level of a general Chem. Phys. course) is recommended. Working knowledge of UNIX/Linux o.s.'s can be useful but it is not required.

1.3.Context and importance of this course in the degree

Molecular Modeling is a 2 ECTS optional subject for the second period of the academic year. This subject is part of the *Structural Characterization* module. As the use of computational chemistry tools is becoming of increasing application in all areas of the chemical sciences it is necessary for the non-specialist to understand the use, application, dificulties an limits of the methods of computational chemistry in the study of chemical compounds and its reactivity.

1.4.Activities and key dates

The information about schedules, calendars and exams is available at the websites of the Sciences Faculty, https://ciencias.unizar.es/calendario-y-horarios, and the Master, http://masterqmch.unizar.es.

Essay presentations will carried out according to the calendar which will be announced in advance.

2.Learning goals

2.1.Learning goals

To understand the computational chemistry methodology used in the study of organic or inorganic molecules and must be able to use them properly in order to analyze the molecular structure, spectrocopic properties and chemical reactivity, including the reaction mechanisms.

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To understand the theoretical component of a theoretical/experimental combined study and assess the relevance of the theoretical part.

To understand the concept of potential energy surface (PES), how it is explored and represented and its relationship whith the reaction mechanism.

To understand the way that molecular orbitals, electron population analysis, electron densities or molecular electrostatic potential can be used in order to interpret the chemical bonding and molecular reactivity.

Understand the role of solvent and solvation on the chemical reactivity and how can be treated from theoretical methods.

To apply computational chemistry concepts to the analysis and problem solution in chemistry and to the comprehension of synthesis, structure and reactivity of molecules.

2.2.Importance of learning goals

The relevance of the acquired competences are a consecuence of the increasing general application in the chemical sciences of computational chemistry along to experimental results.

3.Aims of the course and competences

3.1.Aims of the course

Computational chemistry results are becomming more common in the chemical literature. This subject tries to introduce the student in this methodology. In order to achieve it the neccessary basic theoretical background will be presented which, at least, will enable the students to make a critical understanding of their readings.

An important part is the comprehension of the computational chemistry methodology an in order to grasp it some simple practical applications will be performed.

3.2.Competences

To understand the meaning of the terminology used reporting the results of computational chemistry studies which the students will come accros in the chemical literature.

To know the grounds of the computational chemistry methods which the students will found in the most usual chemical bibliography.

To be able to plan in their work, in an elemental way, the necessary steps to carry out a computational study by themselves or by collaboration with specialists.

To be able to describe in their reports the relevant results to their work found by collaboration with specialists in the field of computational chemistry.

4.Assessment (1st and 2nd call)

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4.1.Assessment tasks (description of tasks, marking system and assessment criteria)

Continous assesment is based on:

1.- Assignements of problems or teoretical-practical questions (20%).

2.- Practical work (computer lab) (20%).

3.- Final exam: problem solution and theoretical-practical questions (60%).

The final mark will be the best of:

0.2*(Problems and questions)+0.2*(Practical work)+0.6*(Final exam) *or* (Final exam)

The number of official examination calls per registration and their use will be subjected to the statements of the *Regulation of Permanence in Master Studies* and the *Regulation of the Learning Assessment* (http://www.unizar.es/ice/images/stories/calidad/Reglamento%20Evaluacion.pdf). The latest document will also regulate the general design and scoring criteria of the assessment activities, as well as the exam schedules and timetable for the post-examination review.

5.Methodology, learning tasks, syllabus and resources

5.1.Methodological overview

he methodology followed in this course is oriented towards achievement of the learning objectives. A wide range of teaching and learning tasks are implemented, such as lectures, problem-solving, and seminars with emphasis on student participation. During the course practical work (computer lab) will be carried out in order to apply the contents of lectures. Finally, in seminars, students with present, analyze, and discuss research papers.

5.2.Learning tasks

The course includes the following learning tasks:

- Lectures (1.2 ECTS).
- Problem-solving sessions and seminars (0.2 ECTS).
- Computer lab sessions (0.6 ECTS).
- Guided assignments.
- Tutorials.

5.3.Syllabus

The course will address the following topics:

Topic 1. Introduction to Computational Chemistry.

Topic 2. Introduction to computational environments and programs of use in chemistry.

Topic 3. The concept of potential energy surface.

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Topic 4. Empirical methods: Molecular mechanics, fundamentals, applications and limits.

Topic 5. Quantum chemistry methods: WFT y DFT.

Topic 6. Analysis of outputs: Study of wavefunction. Molecular properties.

Topic 7. Solvation and solvent effects.

Topic 8. Applications to structural analysis, molecular reactivity and reaction mechanisms.

Topic 9. Use of computational chemistry programs.

5.4.Course planning and calendar

The course runs during the second semester in weekly two-hour sessions. General information about timetables, calendar and exams schedule is available at the Faculty of Science website (https://ciencias.unizar.es).

Handouts and class notes will be available at the reprography services or through the University's virtual platform https://moodle2.unizar.es/add.

5.5.Bibliography and recommended resources

BB Hinchliffe, A. Molecular Modelling for Beginners. 2nd. ed. Wiley. 2008

BB Jensen, Jan H. Molecular modeling basics / Jan H. Jensen Boca Raton, FL [etc.]: CRC Press, 2010

BB Lewars, E. G. Introduction to the Theory and Applications of Molecular and Quantum Mechanics. 2nd. ed. Springer. 2010

BB Rode, Bernd M. The basics of theoretical and computational chemistry / Bernd M. Rode, Thomas S. Hofer and Michael D. Kugler Weinheim: Wiley-VCH, cop. 2007

BC Cramer, Christopher J. Essentials of computational chemistry: theories and models / Christopher J. Cramer . - 2nd ed. Chichester: John Wiley & Sons, 2006

BC Jensen, Frank. Introduction to computational chemistry / Frank Jensen . - 2nd ed. Chichester [etc.]: John Wiley & Sons, cop. 2007