Universidad Zaragoza

Academic Year/course: 2022/23

27230 - Introduction to Molecular Modeling

Syllabus Information

Academic Year: 2022/23
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

2. Learning goals

3. Assessment (1st and 2nd call)

4. Methodology, learning tasks, syllabus and resources

4.1. Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. It favours understanding and scientific reasoning. A wide range of teaching and learning tasks are implemented, such as theory sessions, computer sessions, assignments, computer lab reports, and tutorials.

Students are expected to participate actively in the class throughout the course.

Classroom materials will be available via Moodle. These include lecture notes used in class, the course syllabus, and some other course-specific materials.

Further information regarding the course will be provided on the first day of class.

4.2. Learning tasks

The 5 ECTS course includes the following learning tasks:

- Formative activity 1: Lectures and seminars in order to learn the basic theoretical contents of Molecular Modelling (2.5 ECTS), see section 4.3 for the topics.
- Formative activity 2: Computer lab sessions (0.3 ECTS) for the students to become familiar with the molecular viewer and the calculation programs. The students will work individually, within small groups supervised by the teacher.
- Formative activity 3: Computer lab sessions (2.2 ECTS) on problems or exercises of Molecular Modelling. The students will work individually, within small groups supervised by the teacher. Lab reports will have to be written and presented afterwards.

4.3. Syllabus

The course will address the following tasks:

- **Topic 1. Theory classes: Computational Chemistry Methods.**

- Introduction to Computational Chemistry. Molecular Mechanics or Force Field Methods (MM). Interactions between bonded atoms. Electrostatic interactions and van der Waals Interactions. Force Fields.
- Quantum Chemistry Methods or Electronic Structure Methods (QM). Molecular Orbital Theory. Basis Sets. Hartree-Fock Molecular Orbital Theory. Electron Correlation. Introduction to Density Functional Theory (DFT). Closed-shell Systems and Open-shell Systems.
- Advantages and Limitations of both MM and QM methods. Selection of Level of Calculation. Introduction to Software for Electronic Structure Calculations and for Molecular Visualization. Web Resources. Computer Exercises: Construction of Molecular Structures (Organic and Inorganic).

- **Topic 2. Computer Lab: Practical Application of Molecular Modelling to Problems in Chemistry**
  - Potential Energy Surfaces. Determination of Stationary Points (Minima and Transition States) by Geometry Optimization. Characterization with Frequency Calculation. Methods for the Minimization of the Energy. Strategies for Transition State Searches. Reaction Path, The Intrinsic Reaction Coordinate (IRC). Conformational Analysis, Local and Global Minimal. Determination of Thermodynamic Properties in Model Reactions. Calculation of Kinetic Parameters for Chemical Reactions. Theoretical Calculation of Kinetic Isotope Effects. Other Applications.

4.4. Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course, please refer to the "Facultad de Ciencias" website (https://ciencias.unizar.es).

4.5. Bibliography and recommended resources

http://psfunizar10.unizar.es/br13/egAsignaturas.php?codigo=27230