COURSE DATA

Data Subject	
Code	44975
Name	Methods of theoretical chemistry II
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	2 - Métodos	Obligatory

Coordination

Name	Department
TUÑON GARCIA DE VICUÑA, IGNACIO NILO	315 - Physical Chemistry

SUMMARY

The specific objectives of the course in the form of questions are:

- How can we describe large molecular systems such as proteins or nucleic acids?
- How to describe large molecular systems when a subset of atoms has to be described by quantum mechanics.
- How to describe intermolecular interactions in large systems.
- How to describe molecules in solution.
- Which are the advantadges/disadvantadges of continuum models?
- How to get average and equilibrium properties in systems with many configurations available.
- How can we calculate time-dependent properties.

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

OUTCOMES

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- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- Students should be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- Students should communicate conclusions and underlying knowledge clearly and unambiguously to both specialized and non-specialized audiences.
- Students should demonstrate self-directed learning skills for continued academic growth.
- Students should possess and understand foundational knowledge that enables original thinking and research in the field.
- Students are able to foster, in academic and professional contexts, technological and scientific progress within a society based on knowledge and respect for: a) fundamental rights and equal opportunities between men and women, b) The principles of equal opportunities and universal accessibility for persons with disabilities, and c) the values of a culture of peace and democratic values.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Students are familiar with the fundamental postulates of Quantum Mechanics necessary for a good understanding of the most common methods used in quantum chemistry
- Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- Students understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.

- Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.

LEARNING OUTCOMES

This is the second course of the Master devoted to methods of Theoretical and Computational Chemistry. In this case the focus is on methods for the study of large molecular systems with a large number of accessible conformations. Therefore, the course focuses on three main objectives:

- Calculation of the energy for large systems: force fields, and methods based on continuum models and methods based on the use of hybrid QM / MM potentials
- Exploring the configurational space: Methods of classical and quantum molecular dynamics
- Obtaining dynamic properties through molecular dynamics simulations

DESCRIPTION OF CONTENTS

1.

Intermolecular interactions. Introduction. Long range interactions. Repulsive interactions. Total interactions: models and limitations

2.

Force Fields. Introduction. Energy terms. Parametrization and forcé cfields. Practical questions: validation

3.

Simulation methods. Introduction. Definition of the system. Molecular Dynamics. Practical questions.

4.

Molecular Geometry and Energy. Potential energy surface (PES). Exploration and characterization of stationary points. Molecular properties. Conformational space of biological molecules

5.

Solvation Models applied to Quantum Mechanics. Discrete Models. Continuum Models. Mixed discrete-continuum Models. Hybrid QM/MM Models. Applications

6.

Free Energy Calculations. Introduction. Normal Modes Analysis method. Thermodinamic properties and averaged geometries. Helmholtz and Gibbs Free Energies. Free Energies and Partition Functions. Free Energies as Ensemble Averages. The Particle Insertion Method. Free Energy Perturbation. Thermodynamic Integration. Slow Growth. Umbrella Sampling. Problems and Errors

7.

Advanced Simulation methods: Introduction. Ab Initio Molecular Dynamics. Carr-Parrinello Molecular Dynamics

8.

Advanced Free Energy methods: physical path-based methods: nudged elastic band, dimer method, string method, growing string method, transition path sampling, Parallel Tempering and Replica Exchange MD. History-dependent biasing potential methods: Metadynamics (MTD) and Paradynamics (PD).

9. Laboratory

Practical lesson 1. Calculation of force field terms using quantum mechanics

Practical lesson 2. Molecular Dynamics of aqeuous solutions

Practical lesson 3. Molecular dynamics of proteins

Practical lesson 4. Reactivity: obtaining the reaction profile in gas phase

Practical lesson 5. Reactivity: obtaining the reaction profile in solution

Practical lesson 6. Kinetic isotope effects (KIE).

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	20,00	100
Seminars	15,00	100
TOTAL	35,00	

TEACHING METHODOLOGY

Lecture: The Professor will deliver face-to-face, or, online video lectures about the theoretical contents of the course during two-hour sessions. The presentations will be based on the different materials available at the Moodle platform.

Practical sessions: Teacher will propose exercises based in theoretical concepts seen in lectures to perform calculations with computational programs.

Network teaching: All the tools available at the Moodle website (https://posgrado.uam.es) will be used (uploading of teaching materials, utilization of work team strategies, wiki, blogs, e-mail, etc.).

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

Online Seminars: After the lecturing period, online seminars between the Professor and the students will be arranged at the *virtual classroom* in order to discuss the results being obtained, the potential problems and difficulties in using the various methodologies as well as to supervise the preparation of the required reports

EVALUATION

The knowledge acquired by the student will be evaluated along the course. The educational model to follow will emphasize a continuous effort and advance in training and learning.

The final student mark will be based on exercises that must be done during the course and the discussion of them. These exercises will be based in the contents of practical lessons of the course.

- 70% from the final exam,
- 30% from continuous assesment

Resit

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 70% from the final exam,
- 30% from the individual work.

REFERENCES

Basic

- M. P. Allen, D. J. Tildesley. Computer Simulation of Liquids. Oxford University Press, New York 1989
  A. R. Leach. Molecular Modelling. Longman, London, 1996
  D. Frenkel & B. Smit. Understanding Molecular Simulation. Academic Press, San Diego, 1996
  A. Stone. The Theory of Intermolecular Forces. Oxford University Press, 2013