COURSE DATA

Data Subject	
Code	43993
Name	Methods of theoretical chemistry 2
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

Study (s)

Degree	Center	Acad. year	Period
2184 - Master's Degree in Theoretical Chemistry and Computational Modelling	Faculty of Chemistry	1	Annual
3156 - null		0	First term

Subject-matter

Degree	Subject-matter	Character
2184 - Master's Degree in Theoretical Chemistry and Computational Modelling	2 - Methods	Obligatory

Coordination

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

SUMMARY

English version is not available

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

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

Other requirements

No hay requisitos previos.

COMPETENCES (RD 1393/2007) // LEARNING OUTCOMES (RD 822/2021)

LEARNING OUTCOMES (RD 1393/2007) // NO CONTENT (RD 822/2021)

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

More specifically, 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?

DESCRIPTION OF CONTENTS

1. Unit 1. Intermolecular interactions

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

2. Unit 2. Force Fields

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

3. Unit 3. Simulation methods

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

4. Unit 4 Molecular Geometry and Energy

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

5. Unit 5. Solvation Models applied to Quantum Mechanics

Discrete Models. Continuum Models. Mixed discrete-continuum Models. Hybrid QM/MM Models. Applications

6. Unit 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. Potential of Mean Force. Problems and Errors

7. Unit 7. Advanced Simulation methods

Introduction. Ab Initio Molecular Dynamics. Carr-Parrinello Molecular Dynamics.

8. Unit 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
Development of individual work	30,00	0
Study and independent work	40,00	0
Preparation of practical classes and problem	20,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

Lecture: The Professor will deliver 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.

Network teaching: All the tools available at the Moodle website (http://www.uam.es/moodle) 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

Ordinary assessment

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.

Extraordinary assessment

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