UNIVERSIDAD AUTÓNOMA DE MADRID

32528 - METHODS IN THEORETICAL CHEMISTRY II

Syllabus Information

Code - Course title: 32528 - METHODS IN THEORETICAL CHEMISTRY II

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional
666 -

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Theoretical Chemistry Methods II

1.2.Course nature

651 - Compulsory
666 - Training Supplement
616 - Compulsory

1.3.Course level

666 - Doctorado (MECES 4)
651 - Máster (MECES 3)
616 - Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
666 - : 99
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

Annual

1.6.ECTS Credit allotment

5.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites

1.9.Recommendations

There are no recommendations

1.10.Minimum attendance requirement

Attendance is mandatory

1.11.Faculty data

a. Subject's coordinator:
- Name and surname: Vicent Moliner
- Email: moliner@uji.es
- Institution: Jaume I University
- Department: Physical Chemistry and Analytical Chemistry
- Phone: +34 964728084

b. Lecturer:
- Name and surname: Iñaki Tuñón
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- Institution: University of Valencia
- Department: Physical Chemistry
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c. Master's coordinators:
- Manuel Alcamí. manuel.alcami@uam.es
- Sergio Díaz-Tendero. sergio.diaztendero@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL COMPETENCES

CB6 – Students possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.

CB7 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.

CB8 - Students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments.

CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 - Students possess the learning skills that allow them to continue studying in a way that will be self-directed or autonomous.

CG01 - 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.

CG02 - Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.

CROSS-COMPREHENSIVE COMPETENCES

CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

SPECIFIC COMPETENCES

CE01- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.

CE04 - 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.

CE12 – Students are familiar with the fundamental postulates of Quantum Mechanics necessary for a good understanding of the most common methods used in quantum chemistry.

CE16 - Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem

1.12.2.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

1.12.3.Course objectives

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.

1.13.Course contents

Unit 1. Intermolecular interactions. Introduction. Long range interactions. Repulsive interactions. Total interactions: models and limitations

Unit 2. Force Fields. Introduction. Energy terms. Parametrization and forcé cfields. Practical questions: validation

Unit 3. Simulation methods. Introduction. Definition of the system. Molecular Dynamics. Practical questions.

Unit 4. Molecular Geometry and Energy. Potential energy surface (PES). Exploration and characterization of stationary points. Molecular properties. Conformational space of biological molecules

Unit 5. Solvation Models applied to Quantum Mechanics. Discrete Models. Continuum Models. Mixed discrete-continuum Models. Hybrid QM/MM Models. Applications

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. Umbrella Sampling. Problems and Errors

Unit 7. Advanced Simulation methods: Introduction. Ab Initio Molecular Dynamics. Carr-Parrinello Molecular Dynamics

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).

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).

1.14.Course bibliography

- 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

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	35
Independent study time	90

2.2.List of training activities

Activity	# hours
Lectures	20
Seminars	15
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	
Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

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

3.Evaluation procedures and weight of components in the final grade

3.1.Regular 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.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.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.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	70

Continuous assessment	30

4.Proposed workplan

Please, check the official schedule posted on the master website.