COURSE DATA

Data Subject	
Code	44987
Name	Theoretical methods for simulation of materials
Cycle	Master's degree
ECTS Credits	6.0
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	2	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	4 - Optativas de segundo	Optional

Coordination

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

SUMMARY

The course will focus on the use of theoretical chemistry techniques to describe the properties of new materials. It will include aspects such as the modelling of periodic systems, surfaces, nanotubes, 2D materials such as metal-organic frameworks (COFs), deposition of molecules on surfaces, self-assembly, etc. This type of simulation is at the frontier of physics and chemistry and often requires combining different computational methods to describe both the material and the active part of the material and different effects such as electron transfers. The course will present examples to show how to apply different models and will also include aspects such as the design of materials using machine learning techniques.

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

2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus

- Students should apply acquired knowledge to solve problems in unfamiliar contexts within their field of study, including multidisciplinary scenarios.
- 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 demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Students broaden and/or acquire knowledge of the basic methods of Quantum Chemistry and evaluate its applicability in a critical way.
- Student are familiar with computational techniques which, based on mechanics and molecular dynamics, are the basis for designing molecules of interest in fields such as pharmacology, petrochemistry, etc.
- Students know the existence of advanced computational techniques such as instruction and data channeling, superscalar and multiscalar processors, chain operations, parallel platforms, etc.
- 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 work as a team both at multidisciplinary level and with their own peers respecting the principle of equality of men and women.
- Students are organized at work demonstrating that they know how to manage their time and resources.
- Students are able to generate new ideas based on their own decisions.

LEARNING OUTCOMES

English version is not available

DESCRIPTION OF CONTENTS

1. Theoretical part

1. Nanomaterials: perspective from physics and chemistry.
2. Theory of solids.
3. Design of specific materials.
4. Organic semiconductors for optoelectronics.
5. Organo-inorganic interfaces.
6. Graphene and 2D materials.
7. Functionalisation of graphene and carbon dots.

2. Practical Part

1. VASP
2. Discovering and designing high performance materials.
3. Molecular mechanics/dynamic simulation of molecular materials.
4. Non-periodic DFT calculations of materials and surfaces.

WORKLOAD

ACTIVITY	Hours	% To be attended
Computer classroom practice	20,00	100
Theory classes	20,00	100
Tutorials	5,00	100
TOTAL	**45,00**	

TEACHING METHODOLOGY

English version is not available

EVALUATION

Regular assessment

The final mark for the course will be based on: 20% final exam of the course and 80% corresponding to the delivery of a report of exercises proposed by the professor.

Resit

The evaluation will be based on the delivery of a report with the proposed exercises.

REFERENCES

Basic

- A Computational Chemistry of Solid State Materials. Ronald Holffmann. Wiley-VCH.
  Electronic structure. Basic Theory and Practical Methods. Richard M. Martin.
  Fundamentals of Condensed Matter Physics. Marvin L. Cohen and Steven G. Louie.