VNIVERSITAT DE VALÈNCIA

Course Guide
44989 From theory to implementation: tutorials in theoretical chemistry

COURSE DATA

Data Subject	
Code	44989
Name	From theory to implementation: tutorials in theoretical chemistry
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 aim of this school is to learn how to implement the theory of quantum chemistry in computer code. Therefore, after an introduction to each topic, a lot of time will be spent coding the theory in practical tutorials. Topics include Hückel theory, Hartree-Fock theory, DFT theory, quantum and molecular dynamics, and quantum magnetism.

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 possess and understand foundational knowledge that enables original thinking and research in the field.
- Students handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.
- Students are able to develop efficient programs in FORTRAN in order to use such tools in their daily work.
- Students understand the basic principles of "ab initio" methodologies and Density Functional Theory
- 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 theories and calculation methods for the study of solids and surfaces. Critical evaluation of its applicability to problems of catalysis, magnetism, conductivity, 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 develop a critical thinking and reasoning and know how to communicate them in an egalitarian and non-sexist way both in oral and written form, in their own language and in a foreign language.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- Students have the ability of analyze and synthesize in such a way that they can understand, interpret and evaluate the relevant information by assuming with responsibility their own learning or, in the future, the identification of professional exits and employment fields.
- Students are able to generate new ideas based on their own decisions.
- Students are able to discern between the different existing methods and know how to select the most appropriate method for each problem.

LEARNING OUTCOMES

The aim of this school is to learn how to implement the theory of quantum chemistry in computer code. Therefore, after an introduction to each topic, a lot of time will be spent coding the theory in practical tutorials. Topics include Hückel theory, Hartree-Fock theory, DFT theory, quantum and molecular dynamics, and quantum magnetism.

WORKLOAD

ACTIVITY	Hours	% To be attended
Computer classroom practice	20,00	100
Tutorials	10,00	100
Theory classes	10,00	100
Seminars	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.