COURSE DATA

Data Subject

Code	44991
Name	Multiscale modelling of complex molecular systems
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 main objective of this course is to cover modern methods of ab initio electronic structure theory to investigate the properties of condensed matter in ground, perturbed and excited states. This will be achieved by lectures and exercises (TD), including numerical ones. We will start with Fermi's electron-gas theory, to develop the fundamentals of Density Functional Theory (DFT), the main framework and starting point of modern electronic structure methods. We will evaluate its extension, its main approaches, its operational development and its main applications in the determination of the structural, electronic and magnetic properties of matter in the ground state.

The course will be organized by Sorbonne Univerty.

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 demonstrate self-directed learning skills for continued academic growth.
- 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 handle the most common programming techniques in physics and chemistry and are familiar with the essential computational tools in these areas.
- 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 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.

LEARNING OUTCOMES

English version is not available

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

- Goldstein, Herbert; Poole, Charles; Safko, John. Classical mechanics. 3rd. San Francisco: Addison-Wesley, 2001.

  Lebon, G.; Jou i Mirabent, David; Casas-Vázquez, José. Understanding non-equilibrium thermodynamics: foundations, applications, frontiers. Berlin: Springer, 2008.

  Reichl, L. E. Introduction to modern statistical physics. 3rd rev. and updated ed. Weihheim: Wiley, 2009.

  Sakurai, J. J. ; Napolitano, Jim. Modern quantum mechanics. 2nd ed., international ed. Essex

(England): Pearson, 2014.