VNIVERSITAT DE VALÈNCIA

Course Guide
44984 Advanced methods in electronic structure, dynamics and molecular modelling

COURSE DATA

Data Subject	
Code	44984
Name	Advanced methods in electronic structure, dynamics and molecular modelling
Cycle	Master's degree
ECTS Credits	12.0
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	5 - Métodos y modelización avanzados	Obligatory

SUMMARY

Each year, the course will be organised by one of the universities in the consortium.

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 be able to integrate knowledge and address the complexity of making informed judgments based on incomplete or limited information, including reflections on the social and ethical responsibilities associated with the application of their knowledge and judgments.
- 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 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 understand the basic principles of "ab initio" methodologies and Density Functional Theory
- Students know and critically evaluate the applicability of advanced methods of quantum chemistry to quasi-generated systems, such as systems with transition metals or excited states (their spectroscopy and reactivity).
- 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 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

The course has the following objectives:

- To familiarise students with the possibilities offered by Coupled Cluster methods for the calculation of a variety of molecular properties, essentially representing the response of the molecular system to an electromagnetic perturbation.
- To learn the theoretical basis of the methods, providing information on the plane-wave-pseudopotential method and Fast Fourier Transform techniques.
- Calculation, using DFT methods, of molecular properties of large systems, both for molecules and materials.
- To obtain a theoretical description of the electronic structure that can be used to interpret experimental data, predict interesting phenomena and/or develop new theoretical concepts.
- To introduce the Valence Bond (VB) theory.
- Learn to interpret the results of different Valence Bond calculations using different orbital models. Learn multireference methods.

- Learn to analyse the wave function using different methodologies (AIM, ELF, NBO...).
- Outline the basic principles of the time-dependent wavelet packet approach.
- To know the basics of classical Molecular Dynamics and the steps to prepare MD calculations.
- Time-dependent wave packet approach: obtaining dispersion information.
- Overview of reaction rate theories: the basic properties of elementary reactions obtained from reaction kinetic experiments.
- Familiarity with methods combining classical dynamics with quantum description of parts of the system.
- To know the techniques for coupling electronic and nuclear motion.

DESCRIPTION OF CONTENTS

1. Advanced methods in electronic structure.

- Valence bond theory.
- Electronic correlation with multi-configurational wave function methods.
- Wave function analysis.
- Coupled - Cluster theory.

2. Molecular dynamics and modelling.

- Intramolecular forces.
- Molecular dynamics: fundamentals and simulation of gas physisorption.
- Time-dependent wave packet approach: obtaining dispersion information.
- Ab-initio molecular dynamics: from theory to application.
- QM/MM schemes.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	40,00	100
Computer classroom practice	30,00	100
Seminars	10,00	100
Tutorials	10,00	100
TOTAL	**90,00**	

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

- F Weinhold, C. R. Landis. Valency and Bonding: A Natural Bond Orbital DonorAcceptor Perspective. (Cambridge Univ. Press. 2005)
R. F. W. Bader. Atoms in Molecules. A quantum theory. /Cambridge Univ. Press. 1990).
B. Silvi, A. Savin, Nature 371, 1994, 683.
C. Gatti, P. Macchi, Eds. Modern Charge Density Analysis. (Springer 2012).
Attila Szabo and Neil S. Ostlund, Modern Quantum Chemistry (Macmillan Publishing Co., Inc., 1982).
Trygve U. Helgaker, Poul Jorgensen, and Jeppe Olsen, Molecular Electronic-Structure Theory (John Wiley & Sons Inc., Chichester, 2000).
J. Stone The Theory of Intermolecular Forces, Oxford University Press, 2º Ed. UK. 2013.
Computer simulations of liquids, M.P. Allen and D.J. Tildesley, (Oxford Science Publications, 2000).
D. Marx, and J. Hutter, Ab Initio Molecular Dynamics: Theory and Implementation in Modern Methods and Algorithms of Quantum Chemistry (J. Grotendorst Ed., John von Neumann Institute for Computing, Julich, NIC Series, Vol. 1, pp. 301-449, 2000).