COURSE DATA

Data Subject	
Code	44001
Name	Excited states
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2019 - 2020

Study (s)

Degree	Center	Acad. year	Period
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	Faculty of Chemistry	1	Annual

Subject-matter

Degree	Subject-matter	Character
2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1	5 - Optional subject area	Optional

Coordination

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

SUMMARY

English version is not available

PREVIOUS KNOWLEDGE

Relationship to other subjects of the same degree

There are no specified enrollment restrictions with other subjects of the curriculum.

Other requirements

No pre-requisites

OUTCOMES

2184 - M.U. en Química Teórica y Modelización Computacional 13-V.1

- 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.
- El estudiante es capaz de adaptarse a diferentes entornos culturales.
- Skills in analysis and synthesis.
- Comprender los fundamentos teóricos y prácticos de técnicas con las que puede analizar la estructura electrónica, morfológica y estructural de un compuesto.

LEARNING OUTCOMES

The present course aims to familiarize students with the treatment of both rovibrational and electronic excited states. At the end of the course, the student is expected to know the foundations of the most popular methods and to be able to manage the most frequently used programs for the treatment of excited states.

DESCRIPTION OF CONTENTS

1. Potential energy surfaces

Born-Oppenheimer approximation
Potential energy curves for diatomic molecules
Potential energy surfaces for poliatomic molecules.

2. Interaction radiation-matter

Classical model for electromagnetic radiation
Transition probabilities induced by radiation

3. Rovibrational spectra

Diatomic molecules: energy levels, selection rules.
Pure rotational spectra and rovibrational spectra in diatomic molecules
Polyatomic molecules: classical vibrations and quantum vibrations.
Rovibrational spectra in polyatomic molecules
Vibrational relaxation in liquids: experimental methods and theoretical treatments.

4. Basic Concepts in Modern Molecular Photochemistry

Light absorption: (Electromagnetic radiation, the Lambert-Beer law, Absorption spectra, Franck-Condon principle, Transition dipole moment, Classical and quantum mechanical harmonic oscillator, Selection rules, Electronic transitions)
Deactivation of excited states: (Energy and electron transfer, Jablonski diagrams, Vibrational relaxation, Radiative and non radiative transitions, Franck-Condon principle for radiationless transitions, the Energy gap law, Time scales and quantum yields, Fermis golden rule)
Excited potential energy surfaces: (surface crossings, photochemical reaction paths, Examples).

5. Quantum Chemical Calculations of Excited States: Multiconfigurational Methods.

Electron correlation in molecules.

Electronic Structure methods for excited states. Monoconfigurational vs. multiconfigurational methods. CASSCF and RASSCF methods. Choice of the active space. Single vs. state-average calculations. Basis sets considerations.

Introducing dynamical correlation: the CASPT2 method.

CASPT2 problems and solutions: intruder states, avoided crossings and valence-Rydberg mixing. The level shift technique and Multistate-CASPT2.

Examples.

6. Quantum Chemical Calculations of Excited States: TD-DFT Methods.

DFT, Runge-Gross theorems, linear response TDDFT, propagation of the electronic density.
Spectra calculation, approximation of xc-functionals,
Examples.

7. Dynamics simulations: Wave Packet propagations.

Time-evolution operator, Propagation, Relaxation method, Filtering method. Interaction with an electric field. Correlation functions, Spectra and eigenfunctions. Pump-probe spectroscopy and control.

8. TD-DFT for ultrafast dynamics.

Ab initio molecular dynamics: Born-Oppenheimer and Ehrenfest dynamics. Nonadiabatic dynamics, Tully's surface hopping. Examples of nonadiabatic ab initio molecular dynamics. Addition of environmental effects: Electromagnetic fields and solvents.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	35,00	100
Development of individual work	40,00	0
Study and independent work	50,00	0
TOTAL	**125,00**	

TEACHING METHODOLOGY

Lecture: The Professor will deliver 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.

Network teaching: All the tools available at the Moodle website (http://www.uam.es/moodle) 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.

EVALUATION

Ordinary 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. The next criteria will be followed for assessment of student exercises:

- 60% from the student report about the practical work and/or exercises.
- 40% discussion of the subject during the practical sessions, including a small written test (10%).

Extraordinary assessment

The student will have to face a final exam, including both theory and practical exercises. The student mark will be obtained from:

- 80% from the individual work.
- 20% from the final exam.

REFERENCES

Basic

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  P.F. Bernath, Spectra of Atoms and Molecules (Oxford University Press, Nueva York, 1995).
  J. L. McHale, Molecular Spectroscopy (Prentice Hall, New Jersey, 1999).
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  D.J. Tannor, Introduction to Quantum Mechanics: A Time-Dependent Perspective (University Science Books, 2006).
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N.J. Turro, Modern Molecular Photochemistry (University Science Books, Mill Valley, California, 1991).
B.O. Roos, Ab initio methods in quantum chemistry II in Advances in Chemical Physics, edited by K. P. Lawley (John Wiley & Sons, Inc., 1987), pp. 399445.
edited by M. Olivucci, Computational Photochemistry (Elsevier, Amsterdam, 2005).

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

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