UNIVERSIDAD AUTÓNOMA DE MADRID

31246 - EXCITED STATES

Syllabus Information

Code - Course title: 31246 - EXCITED STATES

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Excited States

1.2.Course nature

Optional

1.3.Course level

Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

651-Annual o First semester
616-Annual o First semester
621-Annual

1.6.ECTS Credit allotment

5.0

1.7.Language of instruction

English

1.8.Prerequisites

There are no previous prerequisites.

1.9.Recommendations

There are no recommendations.

1.10.Minimum attendance requirement

Attendance is mandatory.

1.11.Faculty data

a. Subject's coordinator:
- Name and surname: Jesús González Vázquez
- Email: jesus.gonzalezv@uam.es
- Institution: Universidad Autónoma de Madrid
- Department: Chemistry
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b. Lecturer:
- Name and surname: Adolfo Bastida Pascual
- Email: bastida@um.es
- Institution: University of Murcia
- Department: Physical Chemistry

c. Lecturer:
- Name and surname: Alberto Castro
- Email: acastro@bifi.es
- Institution: BIFI - Institute for Biocomputation and Physics of Complex Systems. University of Zaragoza
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d. Lecturer:
- Name and surname: Daniel Roca
- Email: daniel.roca@uv.es
- Institution: Theoretical Chemistry Group. Institute of Molecular Science (ICMol)

e. Lecturer:
- Name and surname: Lara Martínez Fernández
- Email: lara.martfernandez@gmail.com
- Institution: Universidad Autónoma de Madrid
- Department: Chemistry

f. Lecturer:
- Name and surname: Basile Curchod
- Email: basile.f.curchod@durham.ac.uk
- Institution: Durham University

g. Master's coordinators:
- Manuel Alcamí. manuel.alcami@uam.es
- Sergio Díaz-Tendero. sergio.diaztendero@uam.es

1.12.Competences and learning outcomes

1.12.1.Competences

BASIC AND GENERAL COMPETENCES

CB6 – Students possess and understand knowledge that provides a basis or opportunity to be original in the development and/or application of ideas, often in a research context.

CB7 - Students know how to apply the acquired knowledge and their problem solving capacity in new or little known environments within broader (or multidisciplinary) contexts related to their area of study.

CB9 - Students know how to communicate their conclusions and the knowledge and reasons that support them to specialized and non-specialized audiences in a clear and unambiguous way.

CB10 - Students possess the learning skills that allow them to continue studying in a way that will be self-directed or autonomous.

CG01 - 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.

CG04 - 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.

CROSS-COMPREHENSIVE COMPETENCES

CT03 - 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

SPECIFIC COMPETENCES

CE04 - Students understand the theoretical and practical bases of computational techniques with which they can analyze the electronic, morphological and structural structure of a compound and interpret the results adequately.

CE27 - Students are familiar with the fundamentals of the methods used to treat excited states and are able to handle the most frequently used programs for the treatment of excited states

1.12.2.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.

1.13.Course 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, Fermi's 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

1.14.Course bibliography

- A. Requena y J. Zúñiga, Espectroscopía (Pearson Education, Madrid, 2004).
- P.F. Bernath, Spectra of Atoms and Molecules (Oxford University Press, Nueva York, 1995).
- J. L. McHale, Molecular Spectroscopy (Prentice Hall, New Jersey, 1999).
- J. I. Steinfeld, Molecules and Radiation (The MIT Press, Cambridge, 1989).
- W. S. Struve, Fundamentals of Molecular Spectroscopy (Wiley, Nueva York, 1989).
- S. Svanberg, Atomic and Molecular Spectroscopy (Springer-Verlag, Berlín, 2001).
- J. M. Hollas, Modern Spectroscopy (Wiley, Chichester, 1996).
- I. N. Levine, Molecular Spectroscopy (Wiley, 1980)
- C.A. Ullrich, Time-Dependent Density-Functional Theory: Concepts and Applications (Oxford University Press, USA, 2012).
- D. Marx and J. Hutter, Ab Initio Molecular Dynamics: Basic Theory and Advanced Methods, 1st ed. (Cambridge University Press, Cambridge, 2009).
- D.J. Tannor, Introduction to Quantum Mechanics: A Time-Dependent Perspective (University Science Books, 2006).
- edited by M.A.L. Marques, C.A. Ullrich, F. Nogueira, A. Rubio, K. Burke, and E.K.U. Gross, Time-Dependent Density Functional Theory, 1st ed. (Springer, 2006).
- M.A.L. Marques and E.K.U. Gross, Annual Review of Physical Chemistry 55, 427-455 (2004).
- P.W. Brumer and M. Shapiro, Principles of the Quantum Control of Molecular Processes, illustrated ed. (Wiley-Interscience, 2003).
- L. Serrano-Andrés and M. Merchán, Spectroscopy: Applications in Encyclopedia of Computational Chemistry (John Wiley & Sons, Ltd, 2004).
- S.A. Rice and M. Zhao, Optical Control of Molecular Dynamics, 1st ed. (Wiley-Interscience, 2000).
- edited by B.O. Roos, Lecture Notes in Quantum Chemistry II: European Summer School in Quantum Chemistry, 1st ed. (Springer-Verlag, 1994).
- E.K.U. Gross, J.F. Dobson and M. Petersilka, in Density Functional Theory II, edited by R. Nalewajski (Springer Berlin / Heidelberg, 1996), pp. 81-172.
- 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. 399–445.
- edited by M. Olivucci, Computational Photochemistry (Elsevier, Amsterdam, 2005).

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	# hours
Contact hours (minimum 33%)	35
Independent study time	90

2.2.List of training activities

Activity	# hours
Lectures	35
Seminars	
Practical sessions	
Clinical sessions	
Computer lab	
Laboratory	

Work placement	
Supervised study	
Tutorials	
Assessment activities	
Other	

Lectures: 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 (https://posgrado.uam.es) 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

3.Evaluation procedures and weight of components in the final grade

3.1.Regular 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%).

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	
Continuous assessment	

3.2.Resit

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.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	20
Continuous assessment	80

4.Proposed workplan

Please, check the official schedule posted on the master website.