UNIVERSIDAD AUTÓNOMA DE MADRID

30576 - BASIC REACTION DYNAMICS

Syllabus Information

Code - Course title: 30576 - BASIC REACTION DYNAMICS

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

Dynamics of Chemical Reactions

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. Course Coordinator:
- Name and Surname: Pablo Gamallo
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- Institution: University of Barcelona
- Department: Department of Materials Science and Chemical Physics
- Phone Number: +34 934039308

b. Course Professor:
- Name and Surname: Susana Gómez
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- Institution: University of Salamanca
- Department: Department of Physical Chemistry

c. Course Professor:
- Name and Surname: Xavier Giménez
- Email: xgimenez@ub.edu
- Institution: University of Barcelona
- Department: Department of Materials Science and Chemical Physics

d. Course Professor:
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- Email: fermin.huarte@ub.edu
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e. Course Professor:
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- Institution: University of La Rioja
- Department: Chemistry Department

f. Course Professor:
- Name and Surname: Saulo Vázquez
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- Department: Department of Physicial Chemistry

g. Master's Coordinators:
- Sergio Diaz-Tendero: sergio.diaztendero@uam.es
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Note. The updated complete list of course's professor is published in the website of the institution.

1.12.Competences and learning outcomes

1.12.1.Competences

These learning objectives contribute to provide the following skills for the students:

BASIC AND GENERAL SKILLS

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 SKILLS

CT01 - Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.

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 SKILLS

CE01- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.

CE05 – Students have the ability to handle the main sources of scientific information related to Theoretical Chemistry and Computational Modeling. They are able to search for relevant information in web pages of structural data, physical chemical experimental data, databases of molecular calculations, databases of scientific bibliography and scientific works.

CE26 - Students are able to relate macroscopic observations carried out within the field of Chemical Kinetics with individual collisions taking place at the molecular level.

1.12.2.Learning outcomes

Chemical Reaction Dynamics is the area of science that links the macroscopic measurements performed in the reaction kinetics studies with the individual molecular collisions that are behind any chemical process. The goal of the present course is to provide to the students an overview of this branch of the Chemical Physics. Special emphasis will be put on the following aspects of the subject:

- Relationship between microscopic and macroscopic observables.
- Features, properties and limitations of the theoretical methods most commonly employed in Reaction Dynamics.
- Reaction mechanisms at a molecular level.
- Experimental techniques.

1.13.Course contents

-Molecular reaction dynamics: Introductory concepts of molecular reaction dynamics. Types of molecular collisions. Scattering angle. Reaction rate and cross-section. Excitation function. Opacity function. Differential cross-section. Theoretical methods in collision dynamics: quantum and quasi-classical trajectory (QCT) methods. Experimental observables. Mechanism of reactive collisions. Potential energy surfaces. Examples: Cl + HI, F + H2. Hands-on session.

-Reaction rate theories: Introduction to chemical kinetics. Reaction rate, rate constant, reaction order, and differential rate equations.. Conventional transition state theory (TST): statistical and thermodynamic formulations, calculation of partition functions,. Variational transition state theory (VTST). Tunneling corrections.. Hands-on session: VTST calculations for H + CH3CH2OH -> H2 + CH3CHOH.

-Automated methods for predicting reaction mechanisms. Simulation of coupled chemical reactions by Kinetic Monte Carlo. Hands-on session: Unimolecular decomposition of formic acid.

-Molecular Dynamics: The classical equations of motion. Numerical integration algorithms. Periodic boundary conditions. Types of ensembles. Thermostats and barostats. Force fields: types and their computational cost. Examples. Hands-on session.

-Theoretical study of the mechanism and kinetics of enzyme reactions: Review of quantum mechanics/molecular mechanics (QM/MM) approach. QM/MM potential energy surfaces. QM/MM molecular dynamics: umbrella sampling method. EA-VTST/MT: rate constant calculation in enzyme reactions. Examples: HCV NS3/NS4A protease reactions. Hands-on session.

-Calculating kinetic coefficients of chemical reactions using quantum dynamics: Rate constants from flux correlation functions. Thermal flux eigenstates: physical interpretation. Multiconfigurational time-dependent Hartree method (MCTDH). Benchmark polyatomic calculations. Examples: H +CH4, N + N2.

-Wave-packet quantum dynamics: overview and applications to chemical reactions. Introduction to reaction dynamics. Quantum scattering. Propagators. Observables. S-matrix. Wave-packet. Representations. Hamiltonian. Real wave-packet method. Examples: He + HeH+, Ne + H2+ and H + OH. Hands-on session.

1.14.Course bibliography

1.- “Molecular Reaction Dynamics”, Raphael D. Levine, Cambridge University Press, 2005.
2.- “Tutorials in Molecular Reaction Dynamics”, Mark Brouard and Claire Vallance, Royal Society of Chemistry, 2011.
3.- “Chemical kinetics”, Keith J. Laidler, Harper&Row, 1987
4.- “Theory of Chemical Reaction Dynamics”, Michael Baer (Ed.), Vol IV, CRC Press,1985.

5.- “Molecular collision theory”, M. S. Child, Academic Press, Inc., New York, 1974.
6.- “Understanding molecular simulation”, D. Frenkel and B. Smit, Academic Press, 2002.
7.- "Chemical kinetics", K.J. Laidler, Harper&Row, 1987.
8.-“Introduction to QM/MM simulations”, Gerrit Groenhof in “Methods in Molecular Biology” (Clifton, N.J.) 924, 2013, pg. 43-66.

2.Teaching-and-learning methodologies and student workload

2.1.Contact hours

	#horas
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	

Lecture: The Professor will deliver face-to-face, or, online video 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 teach some subjects and also 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.

Lecture classes in the computing lab: Teaching will be done in a computer lab, Two hours lectures will include an introduction, a theory to introduce the basic concepts and practical work. Student will learn through practicing. During the practical sessions the student will develop his own programs.

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. There will also be an exam at the end. The next criteria will be followed for the assessment of the final mark:

- 80% Completion of requested tasks.

- 20% Final exam.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	20
Continuous assessment	80

3.2.Resit

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

- 50% Final exam.

- 50% Completion of requested tasks.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	50
Continuous assessment	50

4.Proposed workplan

Please, check the oficial master's Schedule published in master's website.