COURSE DATA

Data Subject	
Code	44000
Name	Dynamics of chemical reactions
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2022 - 2023

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.
- Know a foreign language.
- 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.
- El estudiante posee razonamiento crítico.
- Students demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- Manejar las principales fuentes de información científica, siendo capaces de buscar información relevante en internet, de las bases de datos bibliográficas y de la lectura crítica de trabajos científicos.

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.

DESCRIPTION OF CONTENTS

1. 1.-

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

2. 2.-

o 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.
o 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.
o 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.
o 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.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	30,00	100
Other activities	5,00	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.

Lecture classes in the computing lab: Teching 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

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. 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

Extraordinary assessment

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

REFERENCES

Basic

- 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, HarperRow, 1987.
  8.-Introduction to QM/MM simulations, Gerrit Groenhof in Methods in Molecular Biology (Clifton, N.J.) 924, 2013, pg. 43-66.