COURSE DATA

Data Subject	
Code	44977
Name	Dynamics of chemical reactions
Cycle	Master's degree
ECTS Credits	5.0
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	1	Annual

Subject-matter

Degree	Subject-matter	Character
2245 - M.D. in Theoretical Chemistry and Comp.Model.-Erasmus Mundus	3 - Optativas de primero	Optional

SUMMARY

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

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 demonstrate their knowledge and understanding of the facts applying concepts, principles and theories related to the Theoretical Chemistry and Computational Modeling.
- 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.
- Students are able to adapt their selves to different cultural environments by demonstrating that they are able to respond to change with flexibility.
- 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.
- 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.

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.

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	35,00	100
TOTAL	**35,00**	

TEACHING METHODOLOGY

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.

EVALUATION

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.

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.

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.