UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

SYLLABUS DEL CORSO

Chimica Fisica II

2021-2-E2702Q089-E2702Q090M

Aims

The course aims to provide:

- knowledge and understanding of the kinetics of chemical reactions and of introductory elements of quantum chemistry, through lectures.

- ability to apply kinetic principles, through numerous examples presented in class and classroom exercises.

- independent judgment, through the analysis of kinetic problems and the discussion and selection of solutions.

- communication skills, through active participation in lectures and exercises and the oral exam.

- ability to learn, stimulated by the constant effort to resume and integrate the previous knowledge of mathematics, physics and chemistry, useful for the analysis of the structure, properties and chemical reactivity.

Contents

Chemical kinetics: Study of the rates of chemical reactions and rate laws. Reaction mechanisms. Temperature dependence. Catalysis.
Quantum chemistry: Introduction to quantum-mechanics. Applications of quantum chemistry to model systems, atoms and molecules.

Detailed program

Chemical kinetics:

- *Rates of chemical reactions and rate laws. Kinetic experiments.*
- *Methods for determining the order of a reaction and the rate constant.*
- *Elementary stages and multi-stage mechanisms. Identification of the reaction mechanism.*
- *Reaction coordinate, transition state and activation parameters*
- *Arrhenius and Eyring equations.*
- *Catalysis; Michaelis Menten equation.*

Quantum chemistry:

- *Insufficiencies of classical physics for the study of microscopic systems. From classical mechanics to quantum mechanics.*
- *Application of quantum mechanics to model systems (single particle subjected to constrained translational, vibrational and rotational motions).*
- *Introduction to the application of quantum mechanics to the study of atomic structure (hydrogenoid systems and polyelectronic atoms).*
- *Introduction to the application of quantum mechanics to the study of molecular structure (diatomic molecules).*

Prerequisites

Knowledge of general, inorganic and organic chemistry. Basic knowledge of mathematics.

There are no imposed propaedeutics, but it is recommended to have passed the first-year exams and the Physical Chemistry I exam.

Teaching form

Lessons, 7 credits

Exercises, 2 credits

In the Covid-19 emergency period, lessons and exercises will take place remotely asynchronously with

synchronous videoconferencing events.

Textbook and teaching resource

In the e-learning page of the course are provided: the slides presented during the lessons; some exercises with solutions for individual preparation for the written exam.

Recommended text: P. Atkins, J. de Paula, Physical Chemistry, 9th edition

Semester

Second semester

Assessment method

The assessment of the Physical Chemistry II module consists in a written and an oral examinations. The two examinations can be taken separately.
The written examination concerns the solution of problems regarding the Chemical Kinetics and has the objective of verifying the acquired knowledge, the ability to apply this knowledge to the solution of problems, and the ability of judgement. It is evaluated with one of the following judgements: optimum, good, fairly good, sufficient, not admitted. The student who obtains sufficient or an higher evaluation is admitted to the oral examination. The written examination is valid for 6 months.***The oral examination*** includes a brief discussion on the written test and an interview on all the topics covered in class (Kinetics and foundations of Quantum Chemistry). It aims to verify the knowledge and understanding of the exam program and the communication skills.During the Covid-19 emergency period, both tests can be carried out using the WebEx platform and a public link will be provided on the teaching e-learning page for access to the examination of possible virtual spectators.The mark range (18-30/30) is obtained by integrating the evaluations of the written and oral examinations.

The final mark for the course "Physical Chemistry II and Laboratory" is calculated as the weighted average of the evaluations obtained in the two modules "Physical Chemistry II" and "Physical Chemistry Laboratory".

Office hours

Students reception in the office after e-mail appointment.