32524 - STATISTICAL MECHANICS AND SIMULATION APPLICATIONS

Syllabus Information

Code - Course title: 32524 - STATISTICAL MECHANICS AND SIMULATION APPLICATIONS

Degree: 616 - Máster en Química Teórica y Modelización Computacional (2013)
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional
666 -

Faculty: 104 - Facultad de Ciencias

Academic year: 2019/20

1.Course details

1.1.Content area

Statistical Mechanics and Applications on Simulations

1.2.Course nature

651 - Compulsory
666 - Training Supplement
616 - Compulsory

1.3.Course level

666 - Doctorado (MECES 4)
651 - Máster (MECES 3)
616 - Máster (MECES 3)

1.4.Year of study

616 - Máster en Química Teórica y Modelización Computacional (2013): 1
666 - : 99
651 - Máster Erasmus Mundus en Química Teórica y Modelización Computacional: 1

1.5.Semester

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: María Elena Martín Navarro
- Email: memartin@unex.es
- Institution: University of Extremadura
- Department: Chemical Engineering and Physical Chemistry
- Phone: +34 924289300 Ext.: 86125

b. Lecturer:
- Name and surname: José Carlos Corchado Martín-Romo
- Email: corchado@unex.es
- Institution: University of Extremadura
- Department: Chemical Engineering and Physical Chemistry
- Phone: +34 924289300 Ext.: 89787

c. Lecturer:
- Name and surname: Ramón Sayós
- Email: r.sayos@ub.edu
- Institution: University of Barcelona
- Department: Materials Science and Chemical Physics

d. 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.

CB8 - Students are able to integrate knowledge and face the complexity of making judgments from information that, incomplete or limited, includes reflections on social and ethical responsibilities linked to the application of their knowledge and judgments.

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.

CG02 - Students are able to solve problems and make decisions of any kind under the commitment to the defense and practice of equality policies.

CROSS-COMPREHENSIVE COMPETENCES

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

SPECIFIC COMPETENCES

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

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.

CE09 - Students understand the basis of Statistical Mechanics formulated from the collectivities.

CE10 - Students know how to calculate partition functions and apply quantum and classical statistics to the ideal systems of interest in Chemistry.

1.12.2.Learning outcomes

This course is organized in two parts. The first part is dedicated to the foundations of Statistical Mechanics and the second part is devoted to the simulation applications.

After completing the course, the students should understand the central ideas of Statistical Mechanics, formulated on the basis of statistical ensembles. They should understand the main features of the most important ensembles (microcanonical, canonical and grand canonical), and should be able to select the most appropriate ensemble depending on the chemical system that is under investigation. The student should also understand the differences between Fermi-Dirac and Bose-Einstein statistics, as well as the conditions upon which the quantum statistics converge to the classical limit. The student should know how to calculate partition functions and apply quantum and classical statistics to ideal systems of interest in chemistry. The student should understand the differences between real and ideal systems, by analysing the main characteristics of real gases and condensed phases. Moreover, the statistical mechanics of non-equilibrium systems will be treated. Finally and due to the difficulty of finding analytical solutions, simulation methods such as MonteCarlo will be studied to obtain numerical solutions to complex problems.

As applications, students will calculate, making use of the information obtained from first principles through Quantum Chemistry calculation programs (e.g., GAMESS, GAUSSIAN,..) partition functions and enthalpic and entropic corrections to free energy differences in different situations of chemical interest (e.g., thermodynamic equilibrium constants of a gas phase reaction).

In addition, in other applications, different macroscopic properties will be determined by means of simulations with Molecular Dynamics or Monte Carlo methods, using the appropriate force fields to describe the molecular interactions (e.g., TraPPE, GROMOS,..). Examples of some of the applications to be carried out: 1) calculation of a liquid-vapor surface tension (e.g., ethanol), 2) calculation of a liquid-liquid interfacial tension (e.g., dodedane/water), 3) calculation of a diffusion coefficient in a gas mixture (e.g., N_2 and O_2 in air), 4) calculation of an adsorption isotherm for a gas/solid system (e.g., CO_2 on a zeolite).

1.13.Course contents

1- Statistical Mechanics

- Ensembles and postulates of statistical mechanics.
- Microcanonical, canonical and grand canonical ensembles.
- Fermi-Dirac, Bose-Einstein and Boltzmann statistics.
- Classical statistical mechanics. Applications to ideal systems: ideal gases, ideal gas of photons, phonons, electrons in metals.
- Systems of interacting particles: dilute real gases, second virial coefficient, van der Waals equation.
- Statistical mechanics of non-equilibrium systems.
- MonteCarlo simulations.

2- Applications

- Calculation of molecular partition functions and macroscopic properties for a gas-phase reaction (ΔU, ΔS, ΔG, K, ..) at various temperatures.
- Calculation of a liquid-vapor surface tension.
- Calculation of a liquid-liquid interfacial tension.

1.14.Course bibliography

Theoretical and Computational Chemistry: Foundations, Methods and Techniques. J. Andrés y J. Bertrán. Eds. Publ. Univ. Jaime I (Castellón) 2007.

Chandler, D., "Introduction to Modern Statistical Mechanics", (Oxford University Press, London, 1986).

Hill, T. L., “An Introduction to Statistical Thermodynamics” (Dover, New York) 1986.

McQuarrie, D. A., “Statistical Mechanics”, (Harper and Row, New York) 1976.

Toda, M., Kubo, R., Saito, N., "Statistical Physics I, (Spriger-Verlag, Heidelberg) 1992.

Frenkel, D, Smit, B., “Understanding Molecular Simulation” (Academic Press, San Diego), 2002.

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	25
Seminars	
Practical sessions	
Clinical sessions	
Computar lab	10
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.).

Seminars: After the lecturing period, seminars between the Professor and the students are scheduled in order to apply the theoretical contempt to problem solving and to analyze the potential problems and difficulties in using the various methodologies as well as to supervise the preparation of the required reports .

Tutoring sessions: The professor can organize either individual or group tutoring sessions about particular topics and questions raised by students.

Computational laboratory. In several practical sessions the students will make calculations on different macroscopic properties of chemical interest, applying the theoretical knowledge of Statistical Mechanics previously explained.

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% Realization of exercises related to the subject
- 40% Completion of one of the practical sessions carried out in class, and delivery of a critical report on it.

3.1.1.List of evaluation activities

Evaluatory activity	%
Final exam	60
Continuous assessment	40

3.2.Resit

The student will have to face a final exam, including both theory and practical exercises. The latter consists in an individual work that the student will have to do with the programs used during the course.

The student mark will be obtained from:

- 70% from the final exam,
- 30% from the individual work.

3.2.1.List of evaluation activities

Evaluatory activity	%
Final exam	70
Continuous assessment	30

4.Proposed workplan

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