VNIVERSITAT DE VALÈNCIA

Course Guide
43989 Statistical mechanics and applications in simulation

COURSE DATA

Data Subject	
Code	43989
Name	Statistical mechanics and applications in simulation
Cycle	Master's degree
ECTS Credits	5.0
Academic year	2021 - 2022

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	1 - Principles	Obligatory

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.
- 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.
- Comprender los fundamentos teóricos y prácticos de técnicas con las que puede analizar la estructura electrónica, morfológica y estructural de un compuesto.
- Students understand the basis of Statistical Mechanics formulated from the collectivities.
- El estudiante debe saber calcular funciones de partición y aplicar las estadísticas cuánticas y la clásica a los sistemas ideales de interés en Química.
- El estudiante comprende y maneja las herramientas matemáticas requeridas para el desarrollo de la Química Teórica en sus aspectos fundamentales y sus aplicaciones.

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).

DESCRIPTION OF CONTENTS

1. 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. 2- Applications

- Calculation of molecular partition functions and macroscopic properties for a gas-phase reaction (U, S, G, K, ..) at various temperatures.
- Calculation of a liquid-vapor surface tension.
- Calculation of a liquid-liquid interfacial tension.
- Calculation of an adsorption isotherm gas/adsorbing solid

WORKLOAD

ACTIVITY	Hours	% To be attended
Theory classes	25,00	100
Seminars	10,00	100
Development of individual work	30,00	0
Study and independent work	40,00	0
Preparation of practical classes and problem	20,00	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.).

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.

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.

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. The next criteria will be followed for assessment of student exercises:

- 60% Realization of exercises related to the subject.

- 40% fCompletion of one of the practical sessions carried out in class, and delivery of a critical report on it.

Extraordinary assessment

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.

REFERENCES

Basic

- 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

ADDENDUM COVID-19

This addendum will only be activated if the health situation requires so and with the prior agreement of the Governing Council

English version is not available