27213 - Physical Chemistry II

Información del Plan Docente

Academic Year	2017/18
Faculty / School	100 - Facultad de Ciencias
Degree	452 - Degree in Chemistry
ECTS	11.0
Year	3
Semester	Annual
Subject Type	Compulsory
Module	---

1.General information

1.1.Introduction

1.2.Recommendations to take this course

1.3.Context and importance of this course in the degree

1.4.Activities and key dates

2.Learning goals

2.1.Learning goals

2.2.Importance of learning goals

3.Aims of the course and competences

3.1.Aims of the course

3.2.Competences

4.Assessment (1st and 2nd call)

4.1.Assessment tasks (description of tasks, marking system and assessment criteria)

5.Methodology, learning tasks, syllabus and resources

5.1.Methodological overview

The methodology followed in this course is oriented towards achievement of the learning objectives. It favours understanding and scientific reasoning. A wide range of teaching and learning tasks are implemented, such as theory sessions, computer and laboratory sessions, assignments, laboratory reports, and tutorials.

Students are expected to participate actively in the class throughout the course.

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The learning process includes:

Formative activity 1: Lectures on Physical Chemistry (6ECTS), see section 5.3 for the topics.

Formative activity 2: Problem-solving classes and seminars (2 ECTS). A series of problems will be available for the students to work in advance. The classes will take place in small groups; some of the problems will be solved by the teacher, some by the students, and some worked out in groups. In this formative activity is essential the participation of the students.

Formative activity 3: Computer lab sessions (2 ECTS). The students will work individually in Quantum Chemistry exercises, within small groups supervised by the teacher.

Formative activity 4: Laboratory sessions (1 ECTS). The students will carry out lab practices or demonstrations based on Surface Physical Chemistry. In general the students will work in pairs within a small groups supervised by the teacher. Lab reports will have to be written and presented afterwards.

Classroom materials will be available via Moodle. These include lecture notes used in class, the course syllabus, and some other course-specific materials.

Further information regarding the course will be provided on the first day of class.

5.2.Learning tasks

The course includes **11 ECTS** organized according to:

- **Quantum Chemistry (Fundamentals and Atomic Structure)** : 49 hours (35 theory + 14 problems) + 4 hours of computer lab demonstrations.

- Quantum Chemistry (Chemical Bonding) : 8 hours of theory and 16 hours of computer lab.

- Physical Chemistry of Surfaces : 23 hours (17 theory + 6 problems) + 10 hours of lab demonstrations.

5.3.Syllabus

The course will address the following topics:

1. Quantum Chemistry (Fundamentals and Atomic Structure): 49 hours (35 theory + 14 problems) + 4 hours of computer lab demonstrations.

The Origins of Quantum Mechanics . Radiation and Matter: Black Body Radiation. The Photoelectric Effect. The de Broglie Hypothesis. Hydrogen Atom Spectrum and the Bohr Model for the Atom. Heisenberg Uncertainty Principle.

Quantum Mechanics, introduction . Operators. Eigenfunctions and Eigenvalues. The Postulates of Quantum Mechanics. Conservative Systems and Stationary States in Quantum Mechanics. Consequences of Quantum Mechanics Postulates. Expansion of the State Function in Terms of Eigenfunctions. Measurement and the Superposition of States.

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Noninteracting Particles and Separation of Variables. Eigenfunctions of Commuting Operators: Simultaneous and Precise Knowledge of Two Physical Observables. Uncertainty Principle.

Using Quantum Mechanics in simple systems . Particle in a One-dimensional Box. Free Particle in One Dimension. Particle in a Three-dimensional Box. Tunnel Effect. One-dimensional Harmonic Oscillator. Angular Momentum. Rigid Rotor.

The Hydrogen Atom . Solution of the Schrödinger Equation for the Hydrogen Atom. The Hydrogen Atom Orbitals. Spin Angular Momentum. Fine Structure of the Spectrum of the Hydrogen Atom.

Approximate methods . Fundamentals of the Variation Method and the Perturbation Theory. Variation and Perturbation Treatments of the Ground State of Helium, and Comparison between them.

Many electron atoms . Self-Consistent Field Method (Hartree Model). Pauli Exclusion Principle. Slater Determinants. Angular Momentum in Many-electron Atoms. Coupling of Angular Momenta. Atomic Term Symbols. Effect of a Magnetic Field on the Spectral Lines. Normal and Anomalous Zeeman Effect. Hyperfine Structure of Spectral Lines as a Consequence of Isotope Effect and Nuclear Spin.

2. Quantum Chemistry (Chemical Bonding): 8 hours of theory and 16 hours of computer lab

Chemical Bonding: an Introduction to the Theories Proposed to Explain It. The Born-Oppenheimer Approximation. The Hydrogen Molecule Ion H_2^+. Molecular Orbital (MO) Theory. Hydrogen Molecule: Molecular Orbital Theory and Valence-Bond Method (VB). MO Treatment for Homonuclear and Heteronuclear Diatomic Molecules. Polyatomic Molecules.

3. Physical Chemistry of Surfaces: 23 hours (17 theory + 6 problems) + 10 hours of lab demonstrations

Interfaces and Surface Tension. Introduction. The Effect of Curvature on Surface Tension; The Young-Laplace Equation. Capillary Rise. Experimental Methods to Measure Surface Tension. Gibbs Adsorption Isotherm. Monolayer Formation; Detergency.

Adsorption and Heterogeneous Catalysis. Adsorption of Gases on Solid Surfaces. Adsorption Isotherms. Heterogeneous Catalysis.

The Electrified Interface. Structure and Properties. Thermodynamics and Models of Electrified Interfaces. An Introduction to Kinetics of Electrode Reactions. Charge Transfer Overpotential. Diffusion Overpotential. Applications: Electrolytic Deposition and Corrosion of Metals.

5.4.Course planning and calendar

For further details concerning the timetable, classroom and further information regarding this course please refer to the "Facultad de Ciencias" website.

5.5.Bibliography and recommended resources

BB	Atkins, Peter William. Química fisica / Peter Atkins, Julio de Paula . - 8ª ed.

	Buenos Aires [etc.] : Editorial Médica Panamericana, cop. 2008
BB	Bockris, John O'M.. Electroquímica moderna / John O'M. Bockris and Amulya K. N. Reddy ; versión española por José Beltrán Barcelona [etc] : Reverté, D.L.1978-1980
BB	Engel, Thomas. Química física / Thomas Engel, Philip Reid ; capítulo 27, Química computacional, contribución de Warren Hehre ; traducción y revisión técnica, Alberto Requena Rodríguez, José Zúñiga Román, Adolfo Bastida Pascual Madrid [etc.] : Pearson Addison Wesley, D.L. 2006
BB	George, David V.. Principles of Quantum Chemistry . Pergamon Press, 1972
BB	Levine, Ira N.. Fisicoquímica / Ira N. Levine ; traducción, Angel González Ureña ; con la colaboración de Antonio Rey Gayo ... [et al.] . - 5ª ed. Madrid [etc.] : McGraw-Hill, cop. 2004
BB	Levine, Ira N.. Química cuántica / Ira N. Levine ; traducción Alberto Requena Rodríguez, Adolfo Bastida Pascual, José Zúñiga Román . - 5ª ed. Madrid [etc.] : Prentice Hall, D.L. 2001
BB	Química cuántica : Fundamentos y aplicaciones computacionales / Joan Bertran Rusca...[et al.] Madrid : Síntesis, D.L. 2000
BB	Química física / Joan Bertrán Rusca y Javier Núñez Delgado (coords.) Barcelona : Ariel, cop. 2002

Online resources:

	[http://physics.nist.gov/cuu/Constants/]

NIST Chemistry WebBook:
[http://webbook.nist.gov/chemistry/]

[http://physics.nist.gov/cuu/Units/index.html]