Universitat Autònoma de Barcelona

2023/2024

Physics and Chemistry of Surfaces

Code: 103299
ECTS Credits: 6

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OB	3	1

Contact

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Teaching groups languages

You can check it through this link. To consult the language you will need to enter the CODE of the subject.
Please note that this information is provisional until 30 November 2023.

Teachers

Xavier Solans Monfort

Prerequisites

It is recommended to have passed the first full course (Introducció a la Nanociència i la Nanotecnologia, Enllaç Químic i Estructura de la Matèria, i Reactivitat Química) and the followong form the second course: Termodinàmica, Cinètica i Transformacions de Fase, Química Orgànica, Química del Elements i laboratori de microscòpies i caracterització.
It is also recommended to be studying at the same time, or previously, the third year course: Síntesi i Estructura de Materials Cristal·lins i Amorfs.

Objectives and Contextualisation

The objective of this course is to introduce the Surface Science to students, an interdisciplinary science and boundary between physics, chemistry, biology and engineering. The most basic aspects of the chemophysical phenomena that take place at the liquid-gas, solid-liquid, solid-gas and solid-solid interfaces will be treated. Several concepts previously introduced in previous years to students, in course like "Introduction to Nanoscience and Nanotechnology" and "Laboratory of microscopes and characterization of materials" will be deepen in this course. Surface structure of solids as well as their modification, will be studied along with main surface characterization techniques. Surface characterization from a structural, morphological, microstructural and compositional point of view will be described in detail. Knowledge in chemistry and Thermodynamics will be used to address surface phenomena, interface and heterogeneous catalysis, discussing also the different types of catalysts.

Competences

- Adapt to new situations.
- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Apply the general standards for safety and operations in a laboratory and the specific regulations for the use of chemical and biological instruments, products and materials in consideration of their properties and the risks.
- Communicate orally and in writing in one's own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Handle the standard instruments and materials of physical, chemical and biological testing laboratories for the study and analysis of phenomena on a nanoscale.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Operate with a certain degree of autonomy.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.
- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.
- Work on the synthesis, characterisation and study of the properties of materials on a nanoscale from previously established procedures.

Learning Outcomes

1. Adapt to new situations.
2. Apply the acquired theoretical contents to the explanation of experimental phenomena.
3. Communicate orally and in writing in one's own language.
4. Correctly handle standard instruments and materials of physics and chemistry laboratories in nanoscience and nanotechnology.
5. Correctly observe protocols for using instrumentation, reagents and chemical waste in laboratories related to the subject.
6. Critically evaluate experimental results and deduce their meaning.
7. Describe solid and liquid surfaces and the phenomenon of the double layer in loaded interfaces.
8. Describe the mechanisms of surface reactivity and catalysis and distinguish the most important heterogeneous catalysis processes.
9. Draft and present reports on the subject in English.
10. Explain the thermodynamics and kinetics of adsorption.
11. Identify the different types of defect on solid surfaces and recognise the processes of adsorption and modification of surfaces.
12. Identify the thermodynamic and kinetic bases of surfaces and interfaces.
13. Interpret and rationalise the results obtained in the laboratory in processes related with physics and chemistry in nanoscience and nanotechnology.
14. Interpret texts in English on aspects related with the physics and chemistry of nanoscience and nanotechnology.
15. Learn autonomously.
16. Make calculations with chemical reactions or catalysis on surfaces.
17. Make relative correct calculations of the thermodynamics and kinetics of surfaces and interfaces.

18. Manage the organisation and planning of tasks.
19. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
20. Operate with a certain degree of autonomy.
21. Perform and characterise surface modification processes
22. Perform bibliographic searches for scientific documents.
23. Perform reactivity and catalysis tests on surfaces
24. Predict the modification of surfaces on the basis of their composition and the reagents used.
25. Propose creative ideas and solutions.
26. Rationalise the results obtained in the laboratory in terms of physical magnitudes and their relation with the observed physical phenomena.
27. Reason in a critical manner
28. Recognise the risks for the health and environment associated with the manipulation of chemicals and material compounds in general.
29. Recognise the terms used in topics related to nanoscience, nanotechnology and society.
30. Resolve problems and make decisions.
31. Resolve problems with the help of the provided complementary bibliography.
32. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Content

Topic 1. Introduction to surfaces

Topic 2. Structure of solid surfaces

2.1. Basic crystallography in two dimensions (two-dimensional networks, Miller index of crystal planes)

2.2. Notation of surface structures

2.3. Ultra high vacuum and Clean Surfaces

2.4. Atomic structure of clean surfaces (relaxation and reconstruction)

2.5. Atomic structure of surfaces with adsorbate

Topic 3. Surface analytical techniques

3.1. Introduction: Surface sensitivity and surface specificity.

3.2. Diffraction methods (LEED, RHEED)

3.3 AES and XPS electron spectroscopy methods

3.4. Microscopies (AFM, STM, SPM)

Topic 4. Surface phenomena

4.1. Surface tension and surface free energy

4.2. Curved surfaces (Laplace's equation, Kelvin's equation)

4.3. Surface tension measurement methods

Topic 5. Surface tension and interfacial tension

5.1. Surface tension in aqueous solutions

5.2. Gibbs isotherm

5.3. Adhesion work, cohesion work

5.4. Contact angle - Young's equation

5.5. wettability

5.6. Detersion by surfactants

Topic 6. Adsorption phenomena

6.1. Definitions. Gas or vacuum interaction with solids

6.2. Adsorption isotherms (Langmuir isotherm, Temkin isotherm, Freunlich isotherm, BET theory, evaluation of the specific surface, determination of pore size)

Unit 7. Interaction of liquids with solids

7.1. Interfaces loaded.

7.2. Helmholtz-Perrin model

7.3. Gouy-Chapman model

7.4. Stern model

7.5. Electrokinetic phenomena (electrochemistry and corrosion)

Unit 8. Heterogeneous catalysis

8.1. Introduction catalysts Stages of a catalytic process.

8.2. Chemical kinetics in heterogeneous catalysis (temperature influence, Langmuir-Hinshelwood model, Eley-Rideal model)

8.3. Examples of heterogeneous catalysis processes (Cracking. Reforming. Catalytic oxidation)

Methodology

The course consists of: 28 hours of theory + 14 hours of problems + 10 hours of laboratory, per student.

Lectures

They will be carried out combining the use of material in digital format and the board. The teaching staff will present practical cases in order to exemplify the application of various theories and models.

Problem sessions

Participation of the students during the classes of problems will be promoted. Some problem sessions will take place in a group. When the teacher determines it, the delivery of resolved problems will be mandatory. When the teacher determines it, hours of problems can be used to carry out continuous evaluation tests.

Laboratory practices

The practices are compulsory, no unjustified absence will be accepted.

The previous work of reading scripts and revision of the theoretical contents will be fundamental for the good resolution of the problems and the practices.

- Module A will carry out two laboratory practices sessions of 3 hours.

- Module B will hold a practical session of 4 hours and a virtual session of 4 hour (both compulsory).

Tutorials

The faculty staff will be available for consulting queries of students. The use of this didactic resource is strongly recommended.

Annotation: Within the schedule set by the centre or degree programme, 15 minutes of one class will be reserved for students to evaluate their lecturers and their courses or modules through questionnaires.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Practice Activities	10	0.4	1, 2, 15, 6, 3, 21, 22, 16, 17, 18, 13, 14, 4, 19, 20, 24, 25, 26, 27, 23, 29, 9, 32, 5
Problem solving	14	0.56	2, 8, 10, 16, 17, 18, 14, 19, 24, 27, 31, 30, 32
Theory letures	28	1.12	8, 7, 10, 16, 17, 11, 12, 24
tutorized learning	12	0.48	2, 6, 3, 10, 18, 13, 19, 20, 29
Type: Autonomous			
Individual study	36	1.44	1, 2, 15, 6, 8, 7, 10, 22, 18, 11, 12, 20, 25, 27, 9
Practice guides reading and preparation	6	0.24	2, 15, 18
Practice report	12	0.48	2, 6, 3, 22, 16, 17, 18, 13, 14, 19, 24, 25, 26, 27, 29, 9, 32
Problems solving	26	1.04	2, 3, 10, 16, 17, 20, 24, 27, 31

Assessment

The global assessment will be carried out continuously and consists of:
• 2 compulsory partials, with a weight of 40% of the final grade, each.
• 1 delivery of internship reports - in the Chemistry laboratory - whose grade will be 10% of the final grade.
• 1 delivery of practice problems in the classroom in groups, the grade of which will be 10% of the final grade.
• 1 individual delivery of a virtual practice, which does not count towards the final grade but is mandatory and therefore 2 points will be deducted from the overall grade of the subject if the delivery is not made.

Students who have accepted the single assessment modality must:
• compulsory practice in a chemistry laboratory, but you can choose to do the practical problem individually, and you will also have to do the Virtual Practice. The delivery of the corresponding reports can be made up to 48 hours before the day scheduled for the second part of the continuous evaluation.
• carry out a final test of the entire theoretical syllabus and problems of the subject. This test will be carried out on the day on which the students of the continuous assessment take the second part-term.

IMPORTANT: In order to pass the subject, the following two requirements must be met:
• have an overall grade equal to or higher than 5.0 and
• having obtained at least 5.0 points out of 10 in the average of the two partial tests (or of the final test in the case of students who opt for the single assessment).
When the assessment is not passed, breaching one of these two criteria, but a minimum of 3.5 is obtained in the subject as a whole, you will have the right to a written recovery test on the entire syllabus that will allow you to pass the subject with a grade of 5 out of 10.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
First Parcial Test	40	3	0.12	3, 8, 7, 10, 16, 17, 12, 14, 24, 26, 29
Group Problem Solution Report	10	0	0	1, 2, 15, 6, 3, 8, 7, 21, 10, 22, 16, 17, 18, 12, 13, 14, 4, 19, 20, 24, 25, 26, 27, 23, 28, 29, 9, 31, 30, 32, 5
Practice solution report	10	0	0	1, 2, 15, 6, 3, 7, 21, 22, 18, 11, 13, 14, 4, 19, 20, 24, 25, 26, 27, 28, 29, 9, 31, 30, 32, 5
Secon Test	40	3	0.12	2, 3, 7, 11, 12, 14, 24, 27, 29, 30

Bibliography

Surface Analysis -The PrincipalTechniques 2nd Edition Editors JOHN C. VICKERMANManchester Interdisciplinary Biocentre,University of Manchester, U. S. GILMORE National Physical Laboratory, Teddington, UK

https://onlinelibrary-wiley-com.are.uab.cat/doi/book/10.1002/9780470721582

Crystallography and Surface Structure - 2e An Introduction for Surface Scientists and Nanoscientists; By: K. Hermann. *Wiley-VCH Verlag GmBH.* ISBN: 978-3-527-33970-9, 978-3-527-69712-0, 978-3-527-69713-7, 978-3-527-69714-4.

G.T. Barnes, I.R. Gentle, *Interfacial Science: an introduction* (2on ed.), 2010 Oxford University Press, ISBN 978-0-19-657118-5

H.-J. Butt, K. Graf, M.Kappl, *Physics and Chemistry of Interfaces,* 2003 WILEY-VCH Verlag GmbH & Co. ISBN 3-527-40413-9.https://cataleg.uab.cat/iii/encore/record/C__Rb2013137

G. A. Somorjai, *Fundamentos de química de superficies,* versión española de J.A. Rodríguez Renuncio, 1975 Ed. Alhambra

A. J. Bard, L. R. Faulkner, *Electrochemical Methods: Fundamentals and Applications* (2on ed.) 2001 John Wiley and Sons, ISBN: 978-0471043720

Atkins, Peter.; De Paula, Julio. *Química Física*.8ª ed. 2008. Ed. Médica Panamericana. https://cataleg.uab.cat/iii/encore/record/C__Rb2043130

Davis, Mark E. and Davis, Robert J. *Fundamentals of chemical reaction engineering.* Chapter 5 - Heterogeneous Catalysis-. McGraw-Hill Higher Education , New York. (2003). ***http://authors.library.caltech.edu/25070/***

Otero, Enrique- *Corrosión y degradación de materiales*. Editorial Síntesis

Software

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