CÓDE	NAME OF MODULE	TYPE
	ADVANCED THEORETICAL METHODS IN NANOSCIENCE: THEORETICAL METHODS IN GAS/SURFACE DYNAMICS	E

M=mandatory
E = elective

3.3.1. Learning goals of the module.

(List the specific learning goals that the current module should provide to the student; goals can focus on content, skills, or attitudes.)

This module addresses key concepts in the interaction of molecules (gas) with surfaces. The student will learn the fundamentals of molecular structure, electronic properties and chemical processes at surfaces, as well as state of the art theoretical models that are currently used in this researching field. Furthermore, an important goal in this module is that students get practice in the computational methods employed in the simulation of gas/surface interaction dynamics.

3.3.2. Methodology: learning activities and credit value of the module (ECTS).

3.3.2.1. Learning activities.

(Time required to teach the module; links to other modules included in the MSc Program and suggested chronological sequence with the latter)

The module is scheduled for the first term of the second year in the Master's program. The idea is that students have already acquired during the first year all the basic knowledge to follow the concepts and methods given in this module. In particular, the student should be reasonably familiar with quantum mechanics, solid state physics and many-particle physics. The fundamental concepts of these subjects are taught in "Fundamentals of Quantum Mechanics" and "Fundamentals of Solid State Physics", and employed in most of the modules given in the first year of the Master.

The module is divided in a theoretical part, which consists of 25 hours of lectures and seminars, and a practice part of 5 hours. In the theoretical part, the student will learn the basic concepts in molecular structure, electronic and structural properties of surfaces, and the theoretical models employed to describe various properties of interest in the interaction of molecules with surfaces (chemisorption energies, diffusion energies, initial sticking coefficient –dissociative or molecular…). The concepts explained during the lectures and seminars will require 32 hours of student's personal work. The module ends up with the practical part in which the student will learn and practice in computer various codes employed to describe the dynamics of gas(molecules)/surface interactions.

3.3.2.2. ECTS credit value (and time)

1 ECTS credit = 25 hours UPV/EHU

TYPE OF LECTURE(1)	Theory		Practice							Evaluation	
	M(2)	S	PA	PL	PO	TA	TAI	PCL	PCC	Periodic Grading	Final Grading
Classroom ures	15	10			5						3
Personal work (3)	20	12			10						
TOTAL	35	22			15						3

(1) M (standard lecture); S (seminar); PA (practical exercises in classroom); PL (practical exercises in laboratory); PO (practical exercises with computers); TA (non-industrial workshops); TAI (industrial workshops); PCL (clinical practice); PCC (field practice); the acronyms are taken from the Spanish wording.

(2) M = maximum allowed is 60% of the full classroom lectures .

(3) Personal work = time that the student would use to prepare and develop individual and group assignments.

3.3.2.3. Module Program.

(Lectures)

Lecture 1	INTRODUCTION: SURFACE CHEMISTRY AND HETEROGENEOUS CATALYSIS
Lecture 2	MOLECULAR STRUCTURE
Lecture 3	ELECTRONIC AND STRUCTURAL PROPERTIES OF SURFACES
Lecture 4	ELEMENTARY CHEMICAL PROCESSES AT SURFACES
Lecture 5	KINETIC MODELING OF PROCESSES AT SURFACES
Lecture 6	POTENTIAL ENERGY SURFACES
Lecture 7	THEORY OF GAS/SURFACE DYNAMICS
Lecture 8	COMPUTATIONAL METHODS TO SIMULATE GAS/SURFACE DYNAMICS

3.3.2.4. Bibliography.

(Basic and specialized bibliographies, journal references, internet addresses, etc.)

B. H. BRANSDEN AND C. J. JOACHAIM, "PHYSICS OF ATOMS AND MOLECULES", ED. LONGMAN.

JENS. P. DAHL, "INTRODUCTION TO THE QUANTUM WORLD OF ATOMS AND MOLECULES" WORLD SCIENTIFIC.

A. ZANGWILL, "PHYSICS AT SURFACES", CAMBRIDGE UNIVERSITY PRESS.

A. GROSS, "THEORETICAL SURFACE ANALYSIS: A MICROSCOPIC PERSPECTIVE", SPRINGER.

G. A. SAMORJAI, "INTRODUCTION TO SURFACE CHEMISTRY AND CATALYSIS", JOHN WILEY AND SONS.

N. BORTOLAMI, N. H. MARCH, AND M. P. TOSI, "INTERACTION OF ATOMS AND MOLECULES WITH SOLID SURFACES", PLENUM PRESS

3.3.3. Criteria and methods for evaluation and grading

(Analysis of the methodology that will be used to evaluate the learning process of the student)

The method used to evaluate the learning process and the knowledge of the student in this subject will be a final exam that will represent 60% of the final grade. The 40% left will evaluate the student's personal work. In particular, the student will be asked to solve a practical problem using the computational methods explained in the las part of the module.

3.3.4. Learning resources

The student will have access to the bibliographical resources available in the University of the Basque Country, "Centro de Física de Materiales", and "Donostia International Physics Center". Furthermore, the "Donostia International Physics Center" will provide the computational resources neccesary to practice with the various computational methods that are explained in the last part of the module.

3.3.5. Language and number of groups attending the module

1	NUMBER OF GROUPS
x	LANGUAGE: ENGLISH

3.3.6. Fields of science and technology to which the module is related

CODE	FIELD
	PHYSICS OF CONDENSED MATTER
	APPLIED PHYSICS

3.3.7. Department in charge of the Program

CODE	DEPARTMENT (1)
	DEPARTMENT OF MATERIALS PHYSICS

3.3.8. Teachers in charge of the module

DNI	Teacher UPV/EHU	Number of credits
34089368X	Joseba iñaki Juaristi Oliden	1

DNI	Teacher other institutions	Number of credits
16269816F	Maite Alducin Ochoa	1
50836672W	Ricardo Díez Muiño	1