CÓDE	NAME OF MODULE	TYPE
	MODELLING AND MOLECULAR DYNAMICS SIMULATIONS AT THE NANOSCALE	M

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.)

The student should be trained on the basic knowledge about the computer methods of simulation and modelling used at present to study systems of nanometric size.

Moreover, the student should become familiar with the use of standard software packages in which this type of methods are relevant and should master their possible applications and limitations.

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 duration of the subject will be that of a term (four month period), which should correspond to the second of the first year of the degree. The student should have previously attended during the first term (four month period) subjects such as "Fundamentals of Fundamental quantum mechanics" or "Fundamentals of solid state physics", essential for a correct pursuit of the agenda. Generally, the subject will be divided in two great blocks, one due to the simulations of molecular dynamics and a second one aimed to the description of the methods of first principles used in the nano-structure modelling.

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 lectures	15	10			5						
Personal work [3]	20	12			13						
TOTAL	35	22			18						

(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 to ab-initio methods in the modelling of nanostructures
Lecture 2	Solid-state methods
Lecture 3	Quantum chemistry methods
Lecture 4	Introduction to molecular dynamics simulation in the nanoscale
Lecture 5	The concept of forcefield
Lecture 6	Needed algorithms
Lecture 7	Mesoscopic methods

3.3.2.4. Bibliography.

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

- *Computer Simulation of Liquids, M.P. Allen D.J.Tildesley (Oxford Science Punlications, 1987).*
- *Modelling Molecular Structures*, A. Hinchliffe (Wiley and Sons, 2000).
- *Computacional Materials Science*, K. Ohno, K. Esfarjani, and Y. Kawazoe (Springer, Berlin, 1999).
- *Electronic structure: basic theory and practical methods*, Richard M. Martin (Cambridge University Press, 2004)

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 evaluation of the knowledge of the fundamentals obtained by the student will be deduced by means of the individual work, that might include the resolution of practical problems of computer simulation of the structure of systems of nanometric size.

3.3.4. Learning resources

The student should be given open access to the bibliographical material of the libraries of the Faculty of Chemistry of the UPV/EHU, the Unit of Physics of Materials and also to that of the Donostia International Physics Center. Moreover, within the aim of performing computer practices and tasks the computer science resources of the Donostia International Physics Center will be also available.

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
15.976.311 M	Alvarez González, Fernando	1.5

DNI	Teacher other institutions	Number of credits
5277410-Z	Sánchez Portal, Daniel	1.5