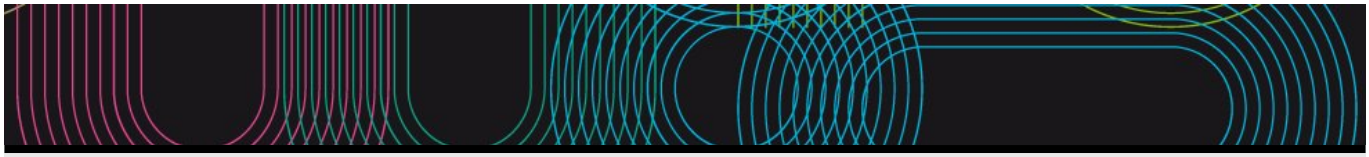
Universidade Vigo

Subject Guide 2023 / 2024



IDENTIFYING DATA				
Computational simulation				
Subject	Computational simulation			
Code	V11M188V01107			
Study programme	Máster Universitario en Nanociencia y Nanotecnología			
Descriptors	ECTS Credits	Choose	Year	Quadmester
	3	Optional	1st	1st
Teaching language	Spanish Galician English			
Department				
Coordinator	Pérez Juste, Ignacio Mandado Alonso, Marcos			
Lecturers	Hervés Beloso, Juan Pablo Mandado Alonso, Marcos Pérez Juste, Ignacio			
E-mail	mandado@uvigo.es uviqpipj@uvigo.es			
Web	http://www.usc.gal/gl/estudos/masteres/ciencias-saude/master-universitario-nanociencia-nanotecnoloxia/20212022/simulacion-computacional-17797-17029-3-98997			
General description	Introduction to the state of the art of computational simulations in nanomaterials, modelling and simulation techniques, and the main computational infrastructures.			

Training and Learning Results
Code

Expected results from this subject	
Expected results from this subject	Training and Learning Results

Contents
Topic
-Introduction to numerical simulation -Classical, semi-clasical and quantum models. -Monte-Carlo simulation techniques -Simulation tools -HPC and HTC approaches

Planning			
	Class hours	Hours outside the classroom	Total hours
Lecturing	10	20	30
Seminars	8	24	32
Laboratory practical	6	7	13
Objective questions exam	0	0	0
*The information in the planning table is for guidance only and does not take into account the heterogeneity of the students.			

Methodologies	
	Description
Lecturing	Presentation by the teacher of the contents on the subject under study, theoretical and / or guidelines for a job, exercise or project to be developed by the student.
Seminars	Activity focused on the work on a specific topic, which allows to deepen or complement the contents of the subject. They can be used as a complement to the theoretical classes.

Laboratory practical	Activities application of knowledge to specific situations and basic skills acquisition and related procedural matter under study. They are developed in specific spaces with specialized equipment (Laboratories, computer rooms, etc ...)

Personalized assistance

Assessment

	Description	Qualification	Training and Learning Results
Seminars	- Active participation in seminars, practical classes and/or oral presentations (40% of the marks). Active participation in seminars and laboratory practices will be evaluated. This evaluation will be carried out by solving questions and problems raised in class, the presentation of works, evaluation tests and/or the participation in the debates.	40	
Objective questions exam	- Written exam on the contents of the subject (60% of the marks). The exam of the subject will consist of short answer questions or tests and / or problems	60	

Other comments on the Evaluation

Sources of information

Basic Bibliography

J. M. Thijssen, **Computational Physics**, Cambridge University Press, 1999

R. M. Martin, **Electronic Structure: Basic Theory and Practical Methods**, Cambridge University Press, 2004

O.C. Zienkiewicz, R.L. Taylor, J.Z. Zhu, **The Finite Element Method: Its Basis and Fundamentals**, Elsevier Butterworth-Heinemann, 2005

P. Pacheco, **An Introduction to Parallel Programming**, Morgan Kaufmann Publishers, 2011

C. J. Cramer, **Essentials of Computational Chemistry: Theories and Models**, 2nd, Wiley, 2005

Complementary Bibliography

Recommendations