SUBJECT TEACHING GUIDE

384 - Simulation and Modelling of New Materials

Master's Degree in New Materials

Academic year 2023-2024

1. IDENTIFYING DATA					
Degree	Master's Degree in New Materials			Type and Year	Optional. Year 1
Faculty	Faculty of Sciences				
Discipline	General Optional Module				
Course unit title and code	384 - Simulation and Modelling of New Materials				
Number of ECTS credits allocated	5	Term		Semester based (2)	
Web					
Language of instruction	Spanish	English Friendly	Yes	Mode of delivery	Face-to-face

Department	DPTO. CIENCIAS DE LA TIERRA Y FISICA DE LA MATERIA CONDENSADA
Name of lecturer	FRANCISCO JAVIER JUNQUERA QUINTANA
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Other lecturers	DIEGO FERREÑO BLANCO EDUARDO OGANDO ARREGUI DAVID DE COS ELICES

3.1 LEARNING OUTCOMES
- Computational simulation of the electronic properties of multielectronic atoms and nanoparticles: binding energy, ground state geometrical configuration, metastable states, electronic density of states, reactivity, electronic bands, vibrational properties... Electronic and structural properties of solids.
- Computational simulation of the macroscopic properties of the bulk materials (elasticity, termal conductivity, ...)
- Approach to the different actual computational methods to tackle with specific problems of the microscopic and macroscopic behavior of the materials.
- Actual use of some of the computer codes for the micro and macro simulation of the properties of the materials.

4. OBJECTIVES

Computational methods for the simulation and modeling of the properties of materials. The students must perform actual simulations.
Elementary description of Density Functional Theory (DFT) as a tool to simulate the quantum electronic properties of any material. Use of different codes to perform the actual calculations: SIESTA-
In the case of macroscopic systems: Use of programs based in the Finite Elements Method (FEM) to solve structural (elasticity and plasticity), electromagnetic and thermal (conduction and convection) problems, and to describe the mutual interplay.
To stress the relevance of these kind of methods in the modern material science. These methods allow for the prediction of the behavior of the materials and they contribute to improve the design of new mechanical or electronic devices.

6. SUBJECT PROGRAM

	CONTENTS
1	Quantum description of electronic systems. Schrödinger equation. Wave function and density.
2	Density Functiona Theory (DFT) Kohn-Sham equations and solving methods. Electronic properties of nanostructured solids using an atomic code and the code SIESTA.
3	Advanced supercomputation applied to the description of the electronic properties of crystals using the Density Functional Method. Use of the code SIESTA.
4	Finite Elements Method (FEM): Modelization and simulation of electromagnetic problems. Programs FEMM and Comsol Multiphysics.
5	Finite Elements Method (FEM) II: Use of the ANSYS code to simulate thermo-mechanical properties (elasticity, plasticity and thermal conductivity)
6	Simulation of Thermomechanical problems II: Elasticity, plasticity and termal conductivity. Electromagnetic problems

7. ASSESSMENT METHODS AND CRITERIA

Description	Type	Final Eval.	Reassessn	%
Paper on simulations on atoms and molecules	Work	No	Yes	30,00
Paper on simulations on solids.	Work	No	Yes	20,00
Paper on simulations with finite element methods.	Work	No	Yes	20,00
Paper on simulations on thermomechanical macroscopic systems.	Work	No	Yes	30,00
TOTAL				100,00

Observations

The professors could propose the modification of the initial versions of the written memories, before the final evaluation.
In order to pass the subject, a threshold mark of 2.0 over 10.0 is required in the four papers.

Observations for part-time students

A report with the results of the simulations. There will be more flexibility with the deadlines to complete the reports.
The reports should include an abstract in English.

8. BIBLIOGRAPHY AND TEACHING MATERIALS
BASIC

1.-) Chapman A.J., “Transmisión de Calor”, 3ª Edición, Editorial Bellisco, 1984, Madrid.
2.-) E. Oñate, B. Suarez, “Aplicaciones del Método de los Elementos Finitos en Ingeniería. Análisis de estructuras” (vol. 1). 477 pp., ISBN: 84-7653-010-2.
3.-) Zienkiewicz O C & Taylor R L. “The finite element method. Vol. I. Basic formulations and linear problems”. London: McGraw-Hill, 1989. 648 p.; Vol. II. “Solid and fluid mechanics: dynamics and non-linearity”. London: McGraw-Hill, 1991. 807 p.
4.-) Stanley Humphries, "Finite-element methods for electromagnetics" (1997) Download at http://www.fieldp.com/femethods.html.
5.-) K. Ohno, K. Esfarjani, and Y. Kawazoe “Computacional Materials Science”, (Springer, Berlin,1999).
6.-) J. M. Thijssen, “Computacional Physics”, Cambridge University Press, Cambridge, 1999.- Daryl L. Logan, “A First Course in the Finite Element Method”, 4ª ed. Cengage-Engineering, 2006.
7.-) Tirupathi R. Chandrupatla and Ashok D. Belegundu, “Introduction to Finite Elements in Engineering”, 3ª ed. Prentice Hall, 2002
8.-) R. G. Parr y W. Yang, ”Density Functional Theory of Atoms and Molecules” (Oxford University Press, 1989)
9.-) J. Kohanoff, "Electronic Structure Calculations for Solids and Molecules. Theory and computational methods", Cambridge U P, Cambridge UK, 2006.
10.-) Richard M. Martin “Electronic structure: basic theory and practical methods”, Cambridge University Press, 2004.
11.-) L. Ramdas Ram-Mohan. “Finite elements and boundary element applications in quantum mechanics”, Oxford University Press, Oxford, 2002. .