Universitat Autònoma de Barcelona

2017/2018

Simulation Techniques

Code: 43440
ECTS Credits: 6

Degree	Type	Year	Semester
4314939 Advanced Nanoscience and Nanotechnology	OT	0	1

Contact

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Use of languages

Principal working language: english (eng)

Teachers

Francesc Torres Canals

Laura Masgrau Fontanet

Prerequisites

Basic notions of quantum mechanics will be required for the ab-initio part of the course.

Objectives and Contextualisation

Introduction to the use of software devoted to the calculation of physical and chemical properties at the nanoscale, and overview of the underlying formalisms.

Skills

- Communicate and justify conclusions clearly and unambiguously to both specialised and non-specialised audiences.
- Continue the learning process, to a large extent autonomously
- Identify the characterisation and analysis techniques typically adopted in nanotechnology and know the principles behind these, within one's specialisation.
- Seek out information in the scientific literature using appropriate channels, and use this information to formulate and contextualise a research topic.
- Show expertise in using scientific terminology and explaining research results in the context of scientific production, in order to understand and interact effectively with other professionals.
- Solve problems in new or little-known situations within broader (or multidisciplinary) contexts related to the field of study.

Learning outcomes

1. Analyse the underlying complexity and the computational limits of the different methods for solving the model's descriptive equations.
2. Communicate and justify conclusions clearly and unambiguously to both specialised and non-specialised audiences.
3. Continue the learning process, to a large extent autonomously

4. Identify the equations governing Newtonian molecular dynamics, the electronic transport of first principles and structural dynamics.
5. Identify the most appropriate computational technique for the problem addressed.
6. Interpret the capacities of a simulation technique and its fundamental limitations on the basis of the terms that the model incorporates.
7. Seek out information in the scientific literature using appropriate channels, and use this information to formulate and contextualise a research topic.
8. Show expertise in using scientific terminology and explaining research results in the context of scientific production, in order to understand and interact effectively with other professionals.
9. Solve problems in new or little-known situations within broader (or multidisciplinary) contexts related to the field of study.
10. Use computational techniques efficiently to study scientific problems relating to materials at the nanoscale.
11. Use simulation tools self-sufficiently to gain greater understanding in experimental situations.

Content

- Brief introduction to Linux.
- Ab-initio methods for electronic transport: Density functional theory. Kohn-Sham equations. Plane waves and quasi-atomic orbitals. Foundations of ballistic transport. Non-equilibrium Green's functions. Getting transmission coefficients with TRANSIESTA - practical sessions: transport through a molecule and graphene nanoribbons.
- Molecular Dynamics with classical force fields: Micro/Macro canonical collectivities, thermostats. Intermolecular forces. Force fields for biological systems. Lammps code - practical sessions: water through a carbon nanotube, and antigen-antibody binding.
- Continuum models: Equations of continuity: mass, momentum, energy. Diffusion, heat conductions, fluids, elasticity. k.p formalism. Elmer Multiphysics code - practical sessions: vibrations in Si nanowires, and flexing of a Si bridge due to thermal dilatation.

Methodology

About 2/5 of the lectures will be traditional lectures, and the remaining 3/5 will be practical sessions using the different software packages. Out-of-class activities will include reading of journal articles, and carrying out small works/simulations expanding what has been explained in class.

Activities

Title	Hours	ECTS	Learning outcomes
Type: Directed			
Traditional lecture	15	0.6	1, 4, 5, 6, 9, 10
Type: Supervised			
Tutorials	22	0.88	1, 3, 4, 6, 10, 11
Type: Autonomous			
Autonomous work	43	1.72	3, 7, 9, 11

Evaluation

A final exam may be required in very specific cases.

Evaluation activities

Title	Weighting	Hours	ECTS	Learning outcomes
Attendance and participation in class	5%-10%	0	0	2, 8
Exposition of a paper	10%-15%	5	0.2	1, 2, 3, 5, 6, 7, 8
Lab reports	70%-85%	65	2.6	1, 2, 3, 4, 5, 6, 7, 8, 9, 10, 11

Bibliography

J. M. Thijssen. Computational Physics (Cambridge University Press, 1999)

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

S. Datta, Electronic transport in mesoscopic systems (Cambridge University Press, 1995)

D. C. Rapaport, The Art of Molecular Dynamics Simulations (Cambridge University Press, 1995)

D. Frenkel, B. Smit, Understanding Molecular Simulations: from algorithms to applications, Academic Press (1996).

O.C. Zienkiewicz, R.L. Taylor and J.Z. Zhu, The Finite Element Method: Its Basis and Fundamentals (6th Ed, Elsevier Butterworth-Heinemann, 2005) **Sections 3.1-3.3**