Universitat Autònoma de Barcelona

2019/2020

Simulation of Nanometric Systems

Code: 103304
ECTS Credits: 6

Degree	Type	Year	Semester
2501922 Nanoscience and Nanotechnology	OT	4	0

Contact

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Use of Languages

Principal working language: spanish (spa)

Some groups entirely in English: No

Some groups entirely in Catalan: No

Some groups entirely in Spanish: No

Teachers

Jordi Faraudo Gener

Prerequisites

It is advisable to have good knowledge of Quantum Mechanics and Solid State Physics.

Basic UNIX knowledge and fundamentals of programming (FORTRAN, python, or C / C ++) are desirable.

Objectives and Contextualisation

Achieve a global vision of simulation methods in nanometric systems, and the possibilities and limitations of each technique. Understand the fundamental principles of the calculation of electronic structure and molecular dynamics algorithms. Introduce the bases of the programming, and get familiar with the general structure of simulation codes, in common scientific programming languages. Apply these computational methods to the study of bio-nano-technological systems. Develop basic skills for the development of a research project, and public exposure of the conclusions of the study.

Competences

- Adapt to new situations.
- Apply the concepts, principles, theories and fundamental facts of nanoscience and nanotechnology to solve problems of a quantitative or qualitative nature in the field of nanoscience and nanotechnology.
- Communicate clearly in English.
- Communicate orally and in writing in ones own language.
- Demonstrate knowledge of the concepts, principles, theories and fundamental facts related with nanoscience and nanotechnology.
- Interpret the data obtained by means of experimental measures, including the use of computer tools, identify and understand their meanings in relation to appropriate chemical, physical or biological theories.
- Lead and coordinate work groups.
- Learn autonomously.

- Manage the organisation and planning of tasks.
- Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
- Operate with a certain degree of autonomy.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse physical, chemical and biological problems in the field of nanoscience and nanotechnology and propose answers or suitable studies for their resolution, including when necessary the use of bibliographic sources.
- Recognise the terms used in the fields of physics, chemistry, biology, nanoscience and nanotechnology in the English language and use English effectively in writing and orally in all areas of work.
- Resolve problems and make decisions.
- Show motivation for quality.
- Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Learning Outcomes

1. Adapt to new situations.
2. Apply Monte Carlo techniques to solve problems in nanotechnology.
3. Apply the acquired theoretical contents to the explanation of experimental phenomena.
4. Apply the concepts of structured and object oriented programming to the development of programs for the simulation and computation of properties on a nanoscale.
5. Communicate clearly in English.
6. Communicate orally and in writing in ones own language.
7. Correctly analyse databases by means of statistical packages.
8. Correctly use archives and libraries of numerical methods to solve linear algebra problems in the simulation of nanometric systems.
9. Critically evaluate experimental results and deduce their meaning.
10. Draft reports on the subject in English.
11. Identify the different paradigms of nanoscale simulation (first principles, semi-empirical methods, continuum methods, molecular dynamics).
12. Identify the situations in which the different methodologies studied can help to resolve problematic situations and know how to select the best techniques.
13. Interpret discrepancies between theoretical and practical results (including simulation) found in measurements.
14. Interpret the capacities of a simulation program in accordance with the terms that the model incorporates and the derived effects.
15. Lead and coordinate work groups.
16. Learn autonomously.
17. Manage the organisation and planning of tasks.
18. Obtain, manage, analyse, synthesise and present information, including the use of digital and computerised media.
19. Operate with a certain degree of autonomy.
20. Perform bibliographic searches for scientific documents.
21. Present brief reports on the subject in English.
22. Propose creative ideas and solutions.
23. Reason in a critical manner
24. Recognise the correct terms for topics related to methodologies and experimentation in nanoscience and nanotechnology.
25. Recognise the range of applicability, both with regard to measurements of the system and the types of computable properties, of these simulation paradigms.
26. Resolve problems and make decisions.
27. Resolve problems with the help of the provided complementary bibliography.
28. Show motivation for quality.
29. Understand texts and bibliographies in English on each of the techniques, methodologies, tools and instruments in the subject area.
30. Use programs for first principle and molecular dynamic calculations.
31. Work correctly with the formulas, chemical equations and magnitudes used in chemistry.

Content

Introduction to programming (7 hours)

Fundamentals of programming (Fortran / python). Modular structure of the programs. Use of variables, functions and subroutines. Use of libraries Introduction to basic algorithms. Boundary conditions. Structure of a Tight-Binding program: Hamiltonian construction, diagonalization and self-consistency. Structure of a simple program of molecular dynamics: search of neighbors, calculation of total energy and forces, equations of movement.

Methods of electronic structure at the nano-scale (9 hours)

Introduction to the simulation of nanosystems. The problem of the electronic structure: the Hartree-Fock approach and the electronic correlations. Fundamentals of the Theory of the Functional of the Density. The equations of Kohn-Sham. The approximation of the pseudopotential. Representations of electronic wave functions. Semi-empirical methods: Tight-Binding. Predictions of material properties.

Atomistic simulation of balanced and equilibrium systems (16 hours)

Fundamentals of the MonteCarlo method and examples. Atomistic modeling: visualization methods, data formats, databases. Atomistic modeling: fundamentals of the Molecular Dynamics method. Molecular Dynamics Ab Initio. Molecular dynamics with force fields. Examples of application to simulation of nanometric systems. Simulation of thermodynamic collectivities: thermostats and barostats. Practical examples of application to bio-nano systems. Use of structural biology database structures for molecular dynamics simulations. Molecular dynamics out of balance: forces and external fields, thermal gradients.

Laboratory demonstrations (20 hours)

Guided computer practices on the different theoretical aspects exposed in the lectures.

Methodology

The training will be based on lectures, classroom problems, and computer lab practices. The student will also have to solve individual problems that will be evaluated, and develop a small group research project, which will be publicly exposed in class.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			
Classroom Practices	7	0.28	1, 7, 4, 16, 29, 6, 28, 20, 17, 12, 18, 19, 22, 23, 24, 10, 27, 26, 31, 8, 30
Lab demonstrations	20	0.8	1, 7, 4, 3, 16, 9, 29, 6, 28, 20, 17, 12, 13, 14, 15, 18, 19, 22, 23, 24, 10, 27, 26, 31, 8, 30
Master Classes	25	1	1, 2, 16, 29, 5, 6, 28, 20, 11, 12, 13, 14, 18, 19, 22, 23, 25, 24, 10, 27, 26
Type: Autonomous			
Final project	25	1	9, 29, 5, 6, 28, 21, 20, 17, 15, 18, 22, 10, 26, 31
Study and problem solving	33	1.32	16, 29, 19, 23, 24, 26

Assessment

The lab demonstrations are mandatory. Continuous evaluation by presenting problems (15%), laboratory practices and reports of them (40%). Small individual projects will be proposed, which will be exposed (preferably in English) as part of the final evaluation (45%).

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Final project	45%	20	0.8	1, 7, 4, 3, 2, 16, 9, 5, 28, 21, 20, 17, 11, 12, 13, 14, 15, 18, 19, 22, 23, 25, 24, 27, 26, 31, 8, 30
Independent problems	15%	10	0.4	16, 29, 6, 28, 20, 13, 19, 22, 23, 27, 26
Lab demonstrations' report	40%	10	0.4	7, 4, 3, 9, 29, 6, 17, 12, 13, 19, 22, 24, 10, 27, 26, 31, 8, 30

Bibliography

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

"Molecular Modelling Basics, Jan H. Hensen, CRC Press, 2010
"Understanding Molecular Simulation", Daan Frenkel y Berend Smit, Academic Press, 2n edition 202

"The Art of Molecular Dynamics Simulation", D. C. Rapaport, Cambridge Univ. Press. 1995.

"Computer Simulations of Liquids", M. P. Allen & D. J. Tildesley, Oxford Univ. Press. 1989.