

Advanced theoretical methods in nanoscience

Description: This course will introduce the student to theoretical methods such as Quantum Chemical Methods and Density Functional Theory (DFT) that are commonly used to study the electronic properties of important systems in Nanoscience. The student will also learn the fundamentals of molecular structure, electronic and structural properties of surfaces and basic concepts on the chemical processes in gas/surface interactions. Furthermore, the student will get practice on the use of computer codes for Quantum Chemical calculations and for DFT calculations (SIESTA and VASP).

Outline:

- 1.- Introduction
- 2.- Molecular Structure
- 3.- Quantum Chemical Methods: Theory.
- 4.- Quantum Chemical Methods: Exercises.
- 5.- Properties of surfaces.
- 6.- Adsorption processes.
- 7.- Density Functional Theory. Theory and Exercises. SIESTA. VASP.

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