Universitat Autònoma de Barcelona

2018/2019

Computational Chemistry of Solids

Code: 102508
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OT	4	2

Contact

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Use of languages

Principal working language: catalan (cat)
Some groups entirely in English: No
Some groups entirely in Catalan: Yes
Some groups entirely in Spanish: No

Prerequisites

There are no prerequisites. However, it is essential that the students has good fundations in quantum chemistry, material science and crystallography.

Objectives and Contextualisation

The Computational Chemistry for Solids Course is designed to introduce to the student to the computer strategies to model and simulate the electronic and spectroscopic properties of simple materials and their surfaces. Also, the course tackles the most usual strategies for modeling the adsorption and reactivity phenomena in heterogeneous solid-gas systems.

For this reason, the first part of the course focuses on presenting the different methods that can be used for calculating the electronic structure (wavefunction based methods, methods based on the Density Functional Theory and molecular mechanics methods). In a second partthe course focusses on the particularities of the modeling of periodical systems, with particular emphasis on the modeling of surfaces and adsorption phenomena.

The general objectives are:

1. Determine the most appropriate level of theory to be used for solving a given case

2. Contrast the advantages and disadvantages of the most common modeling strategies for solids in a given case

3. Design strategies for modeling surfaces and adsorption processes.

4. Apply the most common models of the simulation of materials in simple examples

Content

The course is divided essentially into two parts. A first general part where the most common methods for computing the electronic structure are introduced and a second part detailing the particularities of the modeling of materials and surfaces.

Specifically, the course is divided in nine unites

First part: Foundations of computational chemistry.

1. Introduction to computational chemistry.

2. The Hartree-Fock method

3. Post-Hartree-Fock methods.

4. Methods based on Density functional theory (DFT)

5. Molecular mechanics and QM/MM methods

6. Exploration of the potential energy surface, thermochemistry and solvation.

Second part: Simulation of solids and surfaces.

7. Introduction to solid modeling.

8. Periodical models

9. Modeling of surfaces and adsorption processes.