Universitat Autònoma de Barcelona

2019/2020

Computational Chemistry of Solids

Code: 102508
ECTS Credits: 6

Degree	Type	Year	Semester
2502444 Chemistry	OT	4	0

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

Teachers

Aleix Comas Vives

Prerequisites

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

Objectives and Contextualisation

The Computational Chemistry for Solids Course is an introduction to solid state modeling. The student acquires background on the strategies for modeling the electronic structure of simple materials and their surfaces. Moreover, the course also tackles the most usual strategies for modeling the adsorption and reactivity phenomena in heterogeneous solid-gas and solid-liquid 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 for the modeling of materials in simple examples

Competences

- "Interpret data obtained by means of experimental measures, including the use of IT tools; identify their meaning and relate the data with appropriate chemistry, physics or biology theories."
- Adapt to new situations.
- Apply knowledge of chemistry to problem solving of a quantitative or qualitative nature in familiar and professional fields.
- Be ethically committed.
- Communicate orally and in writing in ones own language.
- Have numerical calculation skills.
- Learn autonomously.
- Manage the organisation and planning of tasks.
- Manage, analyse and synthesise information.
- Obtain information, including by digital means.
- Propose creative ideas and solutions.
- Reason in a critical manner
- Recognise and analyse chemical problems and propose suitable answers or studies to resolve them.
- Resolve problems and make decisions.
- Show an understanding of the basic concepts, principles, theories and facts of the different areas of chemistry.
- Show initiative and an enterprising spirit.
- Show motivation for quality.
- Show sensitivity for environmental issues.
- Use IT to treat and present information.
- Use the English language properly in the field of chemistry.
- Work in a team and show concern for interpersonal relations at work.

Learning Outcomes

1. Adapt to new situations.
2. Analyse the results obtained from calculations during the modelling of solid materials.
3. Analyse the results obtained from catalytic reactions performed in the laboratory.
4. Apply finite models to simple surface chemistry problems.
5. Be ethically committed.
6. Communicate orally and in writing in ones own language.
7. Compare the basic methods of quantum chemistry and molecular mechanics.
8. Construct a representative finite model from the crystalline structure of a solid.
9. Construct a simple surface model from the crystalline structure of a solid.
10. Describe basic computer simulation.
11. Differentiate between the different strategies applied to simulate materials.
12. Distinguish the surface models used to model the behaviour of solids.
13. Have numerical calculation skills.
14. Identify the basic fundaments of modelling solids.
15. Learn autonomously.
16. Manage the organisation and planning of tasks.
17. Manage, analyse and synthesise information.
18. Model simple molecule adsorption processes in known surfaces.
19. Obtain information, including by digital means.
20. Propose creative ideas and solutions.
21. Propose simulations to obtain information on the energy and electronic structure of well described crystalline solids.
22. Read, analyse and extract information from texts in the English language on the different areas of the field of material chemistry.
23. Reason in a critical manner
24. Recognise the basic terms associated to the modelling of solids in the English language.
25. Recognise the strategy for modelling solids applied to examples found in bibliographic sources.
26. Resolve problems and make decisions.
27. Show initiative and an enterprising spirit.
28. Show motivation for quality.
29. Show sensitivity for environmental issues.

30. Use IT to treat and present information.
31. Use computer programs for calculation, simulation and treatment of databases to analyse the structural measurements of materials.
32. Work in a team and show concern for interpersonal relations at work.

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 units

First part: Foundations of computational chemistry.

1. Introduction - the Hartree-Fock method

2. Post-Hartree-Fock methods.

3. Methods based on Density functional theory (DFT)

4. Molecular mechanics and QM/MM methods

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

Second part: Simulation of solids and surfaces.

6. Introduction to solid-state modeling.

7. Periodic models. Real and Reciprocal Space. Blochl Theorem.

8. Band structure and density of states.

9. Modeling of surfaces and adsorption processes. Bonding on surfaces and reactivity.

Methodology

The course is mainly constituted by three different directed activities:

1. The courses where the professor presents and explains the theoretical background of the course, it presents simple examples and key cases are discussed.

2 Sessions in the computer room where simple problems related to the content of the course are tackled in practice.

3. Practical Sessions. In these sessions, students develop a simple project involving the study of the electronic structure of a semiconductor, the modeling of its surfaces and the adsorption of water molecules.

Activities

Title	Hours	ECTS	Learning Outcomes
Type: Directed			

Practical sessions	18	0.72	1, 2, 15, 8, 9, 27, 16, 17, 31, 19, 18, 21, 20, 23, 25, 26, 32, 30
courses	34	1.36	4, 7, 6, 10, 11, 12, 14, 5, 23, 24, 25
Type: Supervised			
Preparing practical sessions	5	0.2	16
Type: Autonomous			
Bibliographic work	6	0.24	2, 15, 6, 27, 12, 16, 17, 22, 19, 20, 24, 25, 26, 32
Preparing oral presentations	5	0.2	27, 28, 17, 19, 20, 26, 32, 30
Study	52	2.08	15, 7, 10, 11, 16, 14, 23, 24, 25
writing of reports and reviews	15	0.6	2, 16, 17, 31, 23, 26, 32

Assessment

The final mark is composed by four different scores:

1. Exams (2 partials or one final that replaces them) that will account for the 60% of the final mark. During the course there will be two partial exams. Each one will be equivalent to 30% of the final mark. It will be necessary to obtain a minimum of 4.5 out of 10 in each exam. The students who do not reach the 4.5 in each partial exam will have to take the final exam to pass the course. This final exam replaces the two partial ones and again at least a 4.5 mark out of 10 is required. Note that, those students that have not performed 2/3 of the continuous evaluation activities will not be allowed to attend the final exam.

2. Analysis of scientific articles (10% of the final mark): During the course two recent scientific articles will be discussed. At the end of the session where the articles are discussed, the students will prepare a report with the main conclusions of the discussion.

3. Reports of the sessions in the computer room (15% of the final mark): There are 5 sessions in the computer room to review and apply the concepts that are being developed in the main courses. These sessions will be evaluated through a brief report that will outline the results and discuss the relationship of the obtained data with the background of the course.

4. Oral presentation of the practical work (15% of the final mark). At the end of the practical sessions there will be an oral presentation in which the results obtained in these sessions will be presented.

Assessment Activities

Title	Weighting	Hours	ECTS	Learning Outcomes
Partial exams	60%	4	0.16	2, 4, 7, 10, 11, 12, 14, 23, 24, 25, 26, 13
Reports associated to the computer room sessions	15%	3	0.12	2, 4, 15, 8, 9, 28, 12, 16, 17, 29, 19, 18, 21, 26, 13, 32, 30
Reviews of bibliographic content	10%	4	0.16	1, 3, 15, 28, 10, 17, 22, 19, 18, 21, 23, 24, 32
practical sessions	15%	4	0.16	2, 4, 7, 6, 8, 9, 27, 28, 10, 14, 31, 5, 18, 21, 20, 23, 26, 13, 32, 30

Bibliography

C.J. Cramer " Essentials of Computational Chemistry: Theory and Models" John Wiley and Sons