

Subject:	<b>COMPUTATIONAL CHEMISTRY</b>
Semester:	<b>Spring</b>
ECTS credits:	<b>2.5</b>
Professors:	<b>Juan Carlos Paniagua</b> <a href="mailto:jpaniagua@ub.edu">jpaniagua@ub.edu</a> <b>Pere Alemany</b> <a href="mailto:p.alemany@ub.edu">p.alemany@ub.edu</a> <b>Antonio Aguilar</b> <a href="mailto:a.aguilar@ub.edu">a.aguilar@ub.edu</a> <b>Josep Maria Bofill</b> <a href="mailto:jmbofill@ub.edu">jmbofill@ub.edu</a>
Department / Faculty:	<b>Dept Química Física</b> <b>Química Orgánica</b> <b>Chemistry - UB</b>

### Objectives:

Know the principal theoretical methods for studying the matter properties and structure at the nanometric scale and be able to apply those methods using computer codes.

### Recommendations / Previous requisites

In order to fully understand the topics in the subject some knowledge of basic quantum mechanics is required. Is strongly recommended to have taken the Quantum Physics and Chemistry of Materials for Nanotechnology subject taught on autumn semester.

### Contents:

#### 1 Polyelectronic systems (16 h)

- 1.1 Introduction to Computational Chemistry.
- 1.2 Variational and perturbational methods.
- 1.3 Hartree-Fock theory. Closed and open shell systems: RHF, ROHF and UHF.
- 1.4 Basis set. The problem of basis set superposition.
- 1.5 Electron density.
- 1.6 Post Hartree-Fock methods.
- 1.7 The DFT method.
  
- 1.8 Exercises and problems.
  - 1.8a The GAMESS code.
  - 1.8b The input structure.
  - 1.8c RHF calculations: Methylene and others.
  - 1.8d UHF calculations: Methylene and others.
  - 1.8e ROHF calculations: Methylene and others.

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- 1.8f RHF+CI calculations: Methylene and others.
- 1.8g MCSCF calculations: Methylene and others.
- 1.8h DFT calculations: Methylene and others.

## **2 The reaction path model (6h)**

- 2.1 The minimum energy path.
- 2.2 The IRC path and other types of path.
  
- 2.3 Exercises and problems.
- 2.3a IRC calculation: The HCN problem.
- 2.3b The gradient extremal calculation: The HCN problem.

## **3 Statistical mechanics (6h)**

- 3.1 The method of Gibbs ensembles.
- 3.2 Microcanonic formalism.
  
- 3.3 Exercises and problems.
- 3.3a The SN2 reactions: The  $\text{Cl}^- + \text{CH}_3\text{Br}$ .

## **Bibliography**

Molecular Modelling principles and applications, Andrew R. Leach, second edition. Prentice Hall, 2001.

Introduction to Quantum Mechanics in Chemistry, Materials Science and Biology. S. M. Blinder. Elsevier, 2004.

Quantum Chemistry and Spectroscopy. Thomas Engel. Pearson Benjamin Cummings, New York, 1996.

### **Plan:**

Lectures:	18 Hours
Laboratory (Computational):	16 Hours
Independent work:	8 Hours
Study:	20 Hours

## **Bibliography**

Molecular Modelling principles and applications, Andrew R. Leach, second edition. Prentice Hall, 2001.

Introduction to Quantum Mechanics in Chemistry, Materials Science and Biology. S. M. Blinder. Elsevier, 2004.

Quantum Chemistry and Spectroscopy. Thomas Engel. Pearson Benjamin Cummings, New York, 1996.

Manual package of GAMESS code.

**Practical sessions:**

Practice 1: Exercices with the GAMESS code.

Practice 2: Reaction Path.

Practice 3: Chemical Reactions and Rate Constants.

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