

APPLIED COMPUTATIONAL CHEMISTRY 2016-2017

Bachelor Degree:	Chemistry		702G
Course title:	Applied Computational Chemistry		537
Year/Semester:	4/2	ECTS Credits:	6,0

DEPARTMENT

Química					
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ENGLISH-FRIENDLY FACULTY

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CONTENTS

- 1.- Basic Quantum Mechanics.
- 2.- The Schrödinger equation for molecules. Born-Oppenheimer approximation.
- 3.- Hartree-Fock method.
- 4.- Post Hartree-Fock methods.
- 5.- Semi-empirical methods.
- 6.- DFT methods.
- 7.- Statistical Mechanics.
- 8.- Molecular Mechanics (MM).
- 9.- Molecular Dynamics (MD).
- 10.- Calculation of molecular properties using MM and MD.
- 11.- Other methodologies of interest in Computational Chemistry.

The course includes a set of computational exercises and projects that introduce and apply the methods discussed in the classes.





REFERENCES

Title

D. A. McQuarrie, Quantum Chemistry 2nd ed., University Science Books (2008)

Christopher J. Cramer, Essentials of Computational Chemistry: Theories and Model, Wiley (2004)

Errol G. Lewars, Computational Chemistry Introduction to the Theory and Applications of Molecular and Quantum Mechanics, Springer (2011)

EVALUATION SYSTEM

Written exams	40%
Classroom participation and discussion	10%
Written reports (practicals)	25%
Projects	25%

A minimum mark of 4.0 points over 10 in the written exams and the written reports is necessary to pass this course.

