COURSE: COMPUTATIONAL CHEMISTRY

STUDIES: 2nd cycle Degree in Chemistry

CODE: 32053

TYPE: O YEAR: 5th TERM: 1
CREDITS (hours/week): 4,5
ECTS CREDITS: 4
PROFESSOR: Jordi Teixidó Closa
LANGUAGE: Catalan

PREREQUIREMENTS: Chemical bond and Matter structure, Linear Algebra, Mathematics, Digital Calculus, Data processing fundamentals, Differential Calculus, Chemiometry, Physical Chemistry (Advanced), inorganic Chemistry, Biochemistry, Organic Chemistry (Advanced)

PREVIOUS KNOWLEDGES: The corresponding to prerequirement courses, in particular the acquired as mathematics, statistics, optimisation, quantum mechanics and spectroscopy fundamentals.

COURSES THAT HAVE TO BE STUDIED SIMULTANEOUSLY:

COURSE DESCRIPTION:

Together with Theory and Experiments, Simulation (modelization) is the third milestone of scientific knowledge. From nineties, the evolution of computers has allowed the useful and effective incorporation of modelization in the chemical environment. Computational Chemistry.
Computational Chemistry is an area of multidisciplinary knowledge. Different areas like Data Processing and Documentation, Mathematics (optimisation, operator algebra, calculus, differential equations, etc.), Physics and Physical Chemistry, Quantum chemistry, biochemistry, organic, inorganic and analytical chemistry and even engineering tend towards it. It is foreseen to give a global view of Chemistry from the perspective of modelization as principal axis of all the knowledges acquired during the studies.

COURSE OBJECTIVES:

1. Give the students the knowledges of Computational Chemistry for the practice of Chemistry [1, 5, 7].
2. Teach to combine the advanced techniques of modelization, characteristic of Chemistry, with the appropriate computational support, as well as to develop simulations that favour the comprehension of theoretical and experimental concepts [1, 2, 3, 5].
3. Teach to analyse and understand phenomena and processes by means of individual or team simulation [2, 3, 5, 7].

CONTENTS:

0.- Introduction
Computational Chemistry. Definition. Classification, Simulation

1.- Computers and graphics.

1.1 Evolution of Data Processing. From PC to supercomputers. Effective calculus. Programs in Computational Chemistry
1.2 Molecular representations 1D, 2D y 3D. Smiles, Z Matrix.
1.3 Visualization. Molecular graphics
1.4 Data base. Substructural searches. Internet

2.- Quantum mechanics.
2.1 Principles of quantum mechanics. Operators
2.2 '*ab initio*' methods Hartree-Fock. Bases. Analysis of orbital populations.
2.3 Post-HF methods
2.4 Semiempyrical methods. Parameterizations

3.- Molecular mechanics
3.1 Field of forces. Parameterisations.
3.2 Mixed methods QM/MM

4.- Optimisation, The problem of minimum. Conformational space. Simulation.
4.1 Optimisation algorithms. Simplex, Steepest Descent, Conjugate Gradient, …
4.2 Reaction coordinates. Transition states
4.3 Conformational analysis. Systematic scanning.
4.4 Random scanning. Montecarlo-Metropolis.
4.5 Molecular dynamics. Ergodic hypothesis.
4.6 Simulated cooling.
4.7 Liquids, solids and solutions.

5.- Molecular properties. Descriptors.
5.1 Observable and non observable
5.2 Geometry. Spectroscopy. Loads,
5.4 Molecular surfaces. Orbitals, maps of electrostatic potential
5.5 2D and 3D descriptors. Fingerprints, topologic, pharmacophore keys, molecular fields
5.6 Analogy (Similitude). Distance.

6.- Chemiometry and QSAR.
6.1 Traditional discovery of drugs. Free-Wilson. Topliss,…
6.2 Rational design. Classical QSAR. Hammett, Hansch,…
6.3 Statistical tools. Multivariate analysis: MLR. PCA, PLS, DA, Clusters,… Validation..
6.4 3D-QSAR. CoMFA/GRID, Pharmacophore
6.5 Direct methods. Docking, Ligand Design, …
6.6 Combinatory Chemistry, Management and selection of literature, Filtering(druglike, admet),…

7.- Real cases and practices.

METHODOLOGY:
On one hand, the course is lectured in master classes in a 50%, where the most relevant parts of the material previously supplied to the student are discussed. There are multimedia and simulation tools that improve the visualization and comprehension of the different subjects. The another 50% of the time is dedicated to practical sessions with personal computer where the student must analyse and solve individually some questions of modelization. At the same time, the student can make additional exercises trying to analyse and solve them individually at home. The objective is that the student consolidates his skill to manage the concepts he has learnt.

EVALUATION:
A. Exams
D. Works done at home
E. Reports
G. Practical works with computer
J. Participation in class

The student must make a scheduled final exam and prepare the reports requested for each of the practical works done in the practical sessions or at home, using the computer. Final qualification is the weighed average sum of the qualifications obtained in the exam, works, reports and participation in class.

CRITERIA FOR RESULTS EVALUATION:

Objective 1:
- The student must show ability to project, differentiate and apply the advanced simulation techniques and use them appropriately to solve chemical problems [A, D, E, G, J].

Objective 2:
- The student must show inductive-deductive skill to understand /solve /discuss multidisciplinary questions and to know how to make use of the appropriate simulation tools [A, D, E, G].

Objective 3:
- The student must show skill to understand /solve /interpret the results obtained in the modelizations [A, D, E, G].

ORDINARY BIBLIOGRAPHY

BIBLIOGRAPHY or COMPLEMENTARY MATERIAL:

Communication, Storage and Retrieval of Chemical Information, *J. Ash, P. Chubb, S. Ward, S. Welford y P. Willett*, Ellis Horwood Ltd., 1985.

Molecular Orbital Theory for organic chemists, *A. Streitwieser, Jr*. John Wiley & sons, 1962

Computational Quantum Chemistry, *A. Hinchliffe*, John Wiley & sons, 1988.

Molecular Quantum Mechanics (2ona. Ed.), *P.W. Atkins*. Oxford University Press, 1989.

Quantum Chemistry (4a. Ed.), *Ira N. Levine*. Prentice-Hall , 1991.

Modern Quantum Chemistry, *Attila Szabo & Neil S. Ostlund*. Macmillan Publishing CO., 1982

Semi-Empirical Methods of Quantum Chemistry, *J. Sadlej*, PWN & Ellis Horwood Ltd., 1985.

A Handbook of Computational Chemistry, *T. Clark*. John Wiley & sons, 1985.

Chemistry by Computer, *S. Wilson*. Plenum Press, 1986.

A Computational Approach to Chemistry, *Dvaid M. Hirst*, Blackwell Scientific Publications, 1990.

Exploring Chemistry with Electronic Structure Methods (2a. Ed.), *James B. Foresman & Æleen Frisch.* Gaussian Inc., 1996.

Computer Simulation Methods, *D.W. Heermann*, Springer-Verlag, 1986.

Lecture Notes in Physics, 258: Molecular Dynamics, W.G. Hoover, Springer-Verlag, 1986.

Proteins: a theoretical perspective of dynamics, structure and thermodynamics, *C.L. Brooks, M. Karplus y B.M. Pettitt*, John Wiley & sons, 1988.

Computational Chemistry, an emphasis on practical calculations, *Milton D. Johnston, Jr.*, Elsevier, 1988.

Chemical Applications of Group Theory (3era. Ed.), *F. Albert Cotton*. John Wiley & sons, 1990.

Chemometrics: a textbook, *D.L. Massart et al.*, Elsevier, 1989.

Mathematical Modeling in Chemistry, Editor: *Paul G. Mezey*. VCH, 1991.

Structure and Reactivity, Editors: *J.F. Liebman y A. Greenberg*, VCH, 1988.

Advances in Molecular Modeling, Editor: *D. Liotta*, Jai Press Inc. 1988 (Vol.1), 1990 (Vol.2).

Reviews in Computational Chemistry, Editors: *K.B. Lipkowitz y D.B. Boyd*, VCH, 1990-

Computational Chemistry using the P.C., D. W. Rogers, VCH, 1990

Exploring Aspects of Computational Chemistry, J.M. Andre et al., Presses Universitaires de Namur, 1997

Química Quàntica, J.C. Paniagua y P. Alemany, Llibres de l'Índex. 1999

Introduction to Computational Chemistry, F. Jensen, Wiley 1999

Química cuántica, J. Beltrán, V. Branchadell, M. Moreno, M. Sodupe, Ed. Síntesis, 2000

Molecular Modelling, Andrew R. Leach, Ed Prentice Hall, 2nd Ed. 2001. ISBN 0-582-38210-6

Essentials of Computational Chemistry, C.J. Cramer, Wiley 2002. ISBN 0-471-48552-7

PREPAIRED BY: Jordi Teixidó Closa

DATE OF THE LAST REVIEW: January 2005