27230 - Introduction to Molecular Modeling

Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	452 - Degree in Chemistry
ECTS	5.0
Course	4
Period	Second semester
Subject Type	Optional
Module	---

1.Basic info

1.1.Recommendations to take this course

1.2.Activities and key dates for the course

2.Initiation

2.1.Learning outcomes that define the subject

2.2.Introduction

3.Context and competences

3.1.Goals

3.2.Context and meaning of the subject in the degree

3.3.Competences

3.4.Importance of learning outcomes

4.Evaluation

5.Activities and resources

5.1.General methodological presentation

5.2.Learning activities

5.3.Program

1.- Theory classes: Computational Chemistry Methods

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Introduction to Computational Chemistry. Molecular Mechanics or Force Field Methods (MM). Interactions between bonded atoms. Electrostatic interactions and van der Waals Interactions. Force Fields.

Quantum Chemistry Methods or Electronic Structure Methods (QM). Molecular Orbital Theory. Basis Sets. Hartree-Fock Molecular Orbital Theory. Electron Correlation. Introduction to Density Functional Theory (DFT). Closed-shell Systems and Open-shell Systems.

Advantages and Limitations of both MM and QM methods. Selection of Level of Calculation. Introduction to Software for Electronic Structure Calculations and for Molecular Visualization. Web Resources. Computer Exercises: Construction of Molecular Structures (Organic and Inorganic).

2.- Computer Lab: Practical Application of Molecular Modelling to Problems in Chemistry

Potential Energy Surfaces. Determination of Stationary Points (Minima and Transition States) by Geometry Optimization. Characterization with Frequency Calculation. Methods for the Minimization of the Energy. Strategies for Transition State Searches. Reaction Path, The Intrinsic Reaction Coordinate (IRC). Conformational Analysis, Local and Global Minima. Determination of Thermodynamic Properties in Model Reactions. Calculation of Kinetic Parameters for Chemical Reactions. Theoretical Calculation of Kinetic Isotope Effects. Other Applications.

5.4.Planning and scheduling

5.5.Bibliography and recomended resources

BB	Jensen, Frank. Introduction to computational chemistry / Frank Jensen . - 2nd ed. Chichester [etc.] : John Wiley & Sons, cop. 2007
BB	Jensen, Jan H.. Molecular modeling basics / Jan H. Jensen Boca Raton, FL [etc.]: CRC Press, 2010
BB	Levine, Ira N.. Química cuántica / Ira N. Levine ; traducción Alberto Requena Rodríguez, Adolfo Bastida Pascual, José Zúñiga Román . - 5ª ed. Madrid [etc.] : Prentice Hall, D.L. 2001
BB	Química cuántica : Fundamentos y aplicaciones computacionales / Joan Bertran Rusca...[et al.] Madrid : Síntesis, D.L. 2000

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BC	Cramer, Christopher J.. Essentials of computational chemistry : theories and models / Christopher J. Cramer . - 2nd ed. Chichester : John Wiley & Sons, 2006
BC	Foresman, J. E.; Frisch, Æ.. Exploring Chemistry with electronic structure methods: A Guide to Using Gaussian. 2nd. ed. Gaussian Inc. 1996
BC	Hinchliffe, A.. Modelling molecular structures. 2nd. Wiley. 2000
BC	Leach, Andrew R.. Molecular modelling : principles and applications / Andrew R. Leach . - 2nd ed. New York : Prentice Hall, 2001

LISTADO DE URL:

Blog: Computational Organic Chemistry (Steven M. Bachrach) - [http://comporgchem.com/blog/]

Blog: Henry Rzepa (Chemistry with a twist) - [http://www.ch.imperial.ac.uk/rzepa/blog/]

Blog: Molecular Modeling Basics - [http://molecularmodelingbasics.blogspot.com.es/]

MolCalc, molecule calculator - [http://molcalc.org/]

Página oficial de Gaussian - [http://www.gaussian.com/index.htm]