60625 - Theoretical and computational chemistry

Información del Plan Docente

Academic Year	2016/17
Academic center	100 - Facultad de Ciencias
Degree	542 - Master's in Chemical Research
ECTS	3.0
Course	1
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

In this subject, the student will learn how to use properly computer programs for the quantum chemical study of molecules (electronic structure methods). Nowadays, molecular computational calculations are a standard tool for chemical research due to the increase of computer performance and friendly user computer codes.

Computational calculations are of high interest in many fields of Chemistry and they are employed to interpret and to understand experimental results, such as obtaining molecular structures, electronic density distribution, to explain the possible reactivity of the molecular or to follow the reaction path, among others. Also they can be used to predict the structure and properties of molecules not yet synthesized in order to guide experimental research.

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5.2.Learning activities

5.3.Program

1- Fundaments of Theoretical and Computational Chemistry

- Introduction to molecular structure. Molecular Orbital Theory. Hückel method: electronic delocalization, resonance energy and aromaticity.

- Hartree-Fock method. Advanced methods: Electronic Correlation and Density Functional Theory. Degenerate electronic systems.

- Basis sets. Calculational methods for molecular properties.

2. Applications of Theoretical and Computational Chemistry.

- Calculation of potential energy surfaces in gas phase.

- Determination of stationary points in complex chemical reactions.

- Theoretical studies of molecular electronic properties.

- Calculation of open shell electronic systems.

- Molecular interactions: hydrogen bonding.

5.4.Planning and scheduling

5.5.Bibliography and recomended resources

- BIBLIOGRAPHY

- Química Cuántica. J. Bertran Rusca, V. Branchadell Gallo, M. Moreno Ferrer, M. Sodupe Roure. Editorial Síntesis 2002.

- Química Cuántica, I. N. Levine. Editorial Prentice may. Madrid 2001.

- Introduction to Computational Chemistry (2nd edition). F. Jensen, John Wiley and Sons, Chichester, 2007.

- Essentials of Computational Chemistry: Theories and Models (2nd edition). C. J. Cramer. John Wiley and Sons, 2004.

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- Molecular Modeling Basics. J. H. Jensen, CRC Press. Boca Raton, 2010

- SPECIALISED BIBLIOGRAPHY

1. (Very avanzed) Química Cuántica Moderna - Szabo Ostlund