UNIVERSITÀ
DEGLI STUDI DI MILANO-BICOCCA

COURSE SYLLABUS

Molecular Modelling

2122-1-F5401Q026

Aims

To present the theoretical basis of quantum mechanical and classical computational methods and their use in the calculation of molecular properties and modeling of molecular processes, providing technical skill in their use by means of computational laboratory experiences.

Knowledge and understanding
At the end of the course the student knows:
- the quantomechanical methods based on the wave function (MO ab initio) and those based on the density functional theory;
- methods for calculating molecular properties;
- molecular simulation methods based on a classical description of molecular systems;
- the potential energy surface and methods for the identification and characterization of stationary points on it.

Applying knowledge and understanding
At the end of the course the student is able to:
- calculate stereo-electronic (geometries, electronic densities, dipole moments) and spectroscopic (infrared spectra) properties of molecular systems;
- sample the (conformational and reactive) potential energy surface both by global methods (molecular dynamics simulations, systematic search techniques) and by local methods.

Making judgements
At the end of the course the student is able to:
- choose the most appropriate calculation method for studying the system of interest;
- identify and calculate the most appropriate molecular properties given the problem to be addressed.

Communication skills
To be able to describe in a technical report in a clear and concise way and to explain orally with a suitable

language the objectives, the procedure and the results of the elaborations carried out.

Learning skills
To be able to apply the acquired knowledge to contexts different from those presented during the course, and to understand the topics covered in the scientific literature concerning the modeling aspects of computational chemistry.

Contents

Quantum mechanical wave function (MO ab initio) and Density Functional Theory methods. Molecular properties calculations. Potential energy surfaces. Molecular Mechanics and simulation methods.

Detailed program

Schrödinger equation for molecular systems and main approximations. MO ab initio methods: the Hartree-Fock method; configuration interaction method and its approximations; the Møller-Plesset (MPn) perturbative methods. Introduction to methods based on the density functional theory. Electron density and derived properties: internal and response electronic properties. Potential energy surface (PES). Definition; conformational analysis. Characterization of stationary points on PES. Stationary points research methods. Vibrational analysis. Thermochemistry analysis. The Molecular Mechanics method. Molecular simulation methods. Monte Carlo and Molecular Dynamics methods. Trajectory analysis.

Computational laboratory experiences include: calculation of electronic energy and molecular properties; calculation of conformational potential energy surface (PES) by means of quantum mechanical (at the HF and correlated methods) and classical methods; calculation of reactive PES by means of quantum mechanical methods; classic molecular dynamics trajectory analysis on a conformational PES; molecular properties of systems in aqueous solution by menas of MD simulations.

Prerequisites

Quantum mechanics theory: principles and applications to atomic and molecular structures. Schroedinger equations, variational method, perturbative method, hydroneoid atoms, many electrom atoms, Born-Oppenheimer approximations, electronic structure of diatomic molecules. Basic concepts of statistical thermodynamics

Teaching form

Teaching includes 3 CFUs (24 hours) of lectures and 3 CFUs (36 hours) of exercises in the computer lab.

During the lab, is assigned to the students, divided into small groups, a problem to be solved using the techniques presented in the lectures. The solution of the problem is guided by the teacher and tends to develop and strengthen the student's ability to identify the most suitable techniques for the application. The methodology useful for producing a report clear in the description of the procedure followed and accurate in presenting the results obtained is also presented.

Textbook and teaching resource

Lecture notes of the teachers: U. Cosentino, G. Moro, C. Greco, D. Pitea *Molecular Modelling*
Videotaping of the lessons on the e-learning page of the course.

Suggested reading:
F. Jensen "*Introduction to computational chemistry*", 2a edizione, Ed. John Wiley & Sons Ltd, 2006.
A.R. Leach: "*Molecular Modelling: Principles and Applications*", Ed. Prentice-Hall, 2001.

Semester

Second semester

Assessment method

The exam consists of two tests. An assessment of the group technical report related to laboratory experiences in terms of completeness, accuracy and clarity. An individual oral interview on the contents of the technical report aimed at verifying: the level of knowledge acquired; the autonomy of analysis and judgment; the student's exhibition skills. The final grade, expressed in thirtieths with possible praise, is given by the average of the two tests.

At request of the student, the exam can be conducted in English.

Office hours

Every day, by appointment