Computational Chemistry (CHIM/02, physical chemistry)

Academic year: 2017-2018
Faculty: Dep. of Chemistry
Study courses: Master degree in chemistry LM-54
Study plans/Curricula: SR: synthesis and reactivity
Type:
Total Credits: 6
Didactic Methods: lessons, direct applications on computers
Didactic Period: first semester
Exam type: thesis and oral presentation
Professor in charge: Fulvio Ciriaco

Training objectives: ability to perform quantum chemistry calculations, to read the output of quantum chemistry suites, to use graphical interfaces to infer and draw results, to understand the limits and strengths of each of the learned methods.

Prerequisites: basis of quantum mechanics, linear algebra (transforms and eigenvalue problems), electrostatics, general chemistry.

Didactic Methods: lessons and contextual application on pcs on free suites and interfaces: NWChem, GAMESS-US, gabedit, avogadro

Course programme
PROGRAMME:
Lectures (24h):
1. mono and plurideterminantal methods
2. electronic correlation
3. perturbative methods and their application to correlation
4. density functional theory
5. perturbative methods for minor contributions to the hamiltonian
6. vibrational and electronic spectra
7. evaluations of potential energy surfaces and their critical points; transition states
8. basis functions; electron core potentials
9. solvent models

Numerical applications (44 h)
1. the hydrogen molecule: HF, DFT and CISD calculation of PES
2. ethanol: HF and DFT minimum energy structure and IR spectrum
3. butadiene: PES characterization and cis/trans transition state evaluation
4. TS for SN1 substitution reactions
5. Diels-Alder reactions, TS finding for concerted reactions
6. octatetraene: UV/VIS spectrum
7. NMR spectrum of ethanol

8. other structures or reactions from already established interests of the participating students

Reference Texts

Notes from the teacher
R. McWeeney: Molecular quantum mechanics
W. Koch, M.C. Holthausen: A chemist's guide to density functional theory
D. McQuarrie, J.D. Simon: Physical chemistry: a molecular approach