QUÍMICA COMPUTACIONAL

This course is a practical introduction to Computational Chemistry with the focus on electronic structure methods, in particular density functional theory (DFT) methods. In the first part of the course the students are familiarized with LINUX and UNIX based operating systems and the common inputstructures used in Computational Chemistry. The second part of the course are practical exercises for single point energy calculations, structure optimizations and molecular property calculations on simple systems. The course finishes with computational projects of 6 weeks in which the students demonstrate their capability to plan and realze the simulation of a “real life” problem. All calculations are performed with the LCGTODFT program deMon2k on stateofthe art LINUX clusters.

Table of Contents

Seminars

- ForceFieldMethods
- SemiempiricalMethods
- DensityFunctionalTheoryMethods
- AbinitioMethods

SuggestedLiterature

demonsoftware
A.M.Köster,P.Calaminici,S.Escalante,R.FloresMoreno,
A.Goursot,S.Patchkovskii,
J.U.Reveles,D.R.Salahub,A.Vela,ThedeMonUser'sGuide,Version1.1(2004)