# *Materia:* COMPUTATIONAL CHEMISTRY

| Duración | Sesiones/semana | Carga semanal | Semestre |
|---|---|---|---|
| 16 semanas | 2 | 3 hrs | Variable |

Profesores que han impartido el curso: *Dr. Andreas M. Köster*

**Propósitos: 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 input structures used in Computational Chemistry. The second part of the course consists of 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 realize the simulation of a "real life" problem. All calculations are performed with the LCGTODFT program deMon2k on state of the art LINUX clusters.**

**Contenidos:**
1 Introduction to LINUX and UNIX.
2 Introduction to deMon2k.
3 Cartesian and Z-Matrix inputs.
4 Basis Sets and Pseudopotentials.
5 Single Point Energy Calculations.
6 Structure Optimization and Frequency Analysis.
7 Molecular Property Calculations.
8 Computational Projects.
9 Seminars:

- Force Field Methods.
- Semiempirical Methods.
- Density Functional Theory Methods.
- Ab-initio Methods.

Suggested Literature:

A.M.Köster, P.Calaminici, S.Escalante, R.FloresMoreno, A.Goursot, S.Patchkovskii,J.U.Reveles, D.R.Salahub, A.Vela, The deMon User's Guide, Version1.1 (2004)