QUÍMICA TEÓRICA I

This course gives an introduction to Theoretical Chemistry with the focus on variational methods. In the first part of the course Theoretical Chemistry I the Hartree-Fock method is derived within the framework of molecular orbital theory. For the inclusion of correlation the configuration - interaction (CI) approach is discussed. In a next step the Kohn-Sham equations are derived in the framework of the linear combination of Gaussian type orbitals. The aim of this first part of the course is to familiarize the students with various standard methodologies in Theoretical Chemistry and the corresponding mathematical techniques. The second part of the course focuses on first-principle molecular integral approximations and their practical implementation. The aim of this part of the course is to provide the theoretical background for the integral approximations used in modern electronic structure codes, like deMon2k.

Table of Contents

- Born-Oppenheimer Approximation
- Atomic Units
- The Antisymmetry Principle
- The MO-LCAO Approximation
- Molecular Hartree-Fock Method
- Molecular Configuration-Interaction
- Molecular Kohn-Sham Method
- Variational Fitting of the Coulomb Potential
- Auxiliary Density Functional Theory
- Calculation of Molecular Integrals

Suggested Literature:

- F.L. Pilar, Elementary Quantum Chemistry, 2Actualizarnd Edition (McGraw-Hill, New York, 1990)
- A. Szabo, N .S. Ostlund, Modern Quantum Chemistry (Dover Publications, New York, 1996)
- T. Helgaker, P. Jorgensen, J. Olsen, Molecular Electronic Structure Theory (Wiley, New York, 2000)