Course on the Amsterdam Density Functional Program in September 2013

Date		Lectures/ laboratories	Teachers	Subject
23.09.2013	11:15-13:00	lect.	CFG	Introduction: Quantum Chemistry and ADF
	14:15-17:00	lab.	CFG	Tutorial, Basis sets and Molecular Orbitals
24.09.2013	11:15-13:00	lect.	FMB	From hydrogen atom to Hartree-Fock
	14:15-17:00	lab.	CFG	Tautomerization and rotation barriers in gas phase and solvents
25.09.2013	11:15-13:00	lect.	FMB	From Hartree-Fock to DFT
	14:15-17:00	lab.	CFG	Choosing a functional in DFT calculations and SN2 Reaction Profiles
26.09.2013	11:15-13:00	lect.	FMB	Kohn-Sham MO Theory
	14:15-17:00	lab.	CFG	Energy decomposition analyses and MO interaction diagrams

Lectures : Audytorium Zawadzkiego, Faculty of Chemistry, Noakowskiego Street 3, Warsaw
Laboratories: lecture hall no. 130, Chemical Technology Building, Koszykowa Street 75, Warsaw

CFG - dr Cealia Fonseca Guerra
FMB - prof. F. Matthias Bickelhaupt

Goal

Computational chemistry plays a central role in modern chemical research. Various molecular properties can be computed with chemical accuracy. In this way, information can be obtained about quantities that are experimentally inaccessible yet indispensible for molecular design and synthesis. One of the main objectives of this course is to learn current state-of-the-art quantum chemical methods and Amsterdam Density Functional computer software. This course deals with ab initio theory (among others, Hartree-Fock and Møller-Plesset theory) and modern density functional theory (DFT).

These methods are applied in a computer lab in order to get acquainted with important modeling skills, such as, geometry optimization (molecular structure, stability, and thermochemistry), the exploration of potential energy surfaces (kinetics, reaction mechanism) and molecular orbital (MO) theory.
An important issue in this course is the unifying power of computational chemistry: the same theoretical models serve as tools for solving very diverse problems from all branches of chemistry, ranging from organic chemistry and catalysis via biochemistry till pharmaceutical sciences.

The course is intended for PhD students (and master students). The aim is to provide participants with enough background and hands-on experience to get started in modeling chemical structures and reactions with the Amsterdam Density Functional Program. Theoretical background is provided, but the emphasis is on the application of computational methods to help in answering questions in chemical research.

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